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Ferro- and Antiferroelectric Substances

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II Data

Oxides

1 Perovskite-type oxides

1A Simple perovskite-type oxides

Nr. 1A-1 NaNbO₃, Sodium niobate

a	It was reported by MATTHIAS et al. in 1951 that NaNbO ₃ was ferroelectric. Cross et al., however, proved in 1955 that at room temperature it is not ferroelectric but antiferroelectric.						51M2 55C2
b	phase	V	IV	III*	II	I	
	state	F	A			P	
	crystal system	monoclinic	orthorhombic	pseudo-tetragonal	tetragonal	cubic	*61W2 58R3
	space group		Pbma ^a -D _{2h} ¹¹			Pm3m-O _b ¹	
	Θ^{**}	-200	354	562	640	°C	
	$P_s \parallel [001]$ in phase V. Phase IV: $a = 5.568 \text{ \AA} (\cong \sqrt{2}a_0)$, $b = 5.505 \text{ \AA} (\cong \sqrt{2}a_0)$, $c = 15.518 \text{ \AA} (\cong 4a_0)$, where a_0 is the lattice constant of the cubic cell of phase I. In phase IV (orthorhombic system) the longest edge of a unit cell is taken as the c axis (see Fig. 1). This system of the axes is adopted here. In Well and Megaw's analysis b and c axes were interchanged. The orthorhombic structure is also represented by a pseudomonoclinic unit cell (see Fig. 1), where $b' = c$, $a' = c' (\cong a_0)$, $\beta' \cong \pi/2$.						51V3
2a	Cooling method from a molten mixture of Na ₂ CO ₃ , Nb ₂ O ₅ , and NaF.						61W2 51W1
3	Crystal structure: In phase IV, $Z = 8$. Tab. 1; Fig. 1, 2.						
4	Lattice distortions (thermal expansion): For phase I, II, III, IV: Tab. 2, 3; Fig. 3. For phase V, at -160 °C: $a = 5.564 \text{ \AA} (\cong \sqrt{2}a_0)$, $b = 5.548 \text{ \AA} (\cong \sqrt{2}a_0)$, $c = 7.812 \text{ \AA} (\cong 2a_0)$, $\beta = 91^\circ 09'$. Fig. 4.						57J1
5a	Dielectric constants: Fig. 5. Curie-Weiss law: $\kappa = C/(T - \Theta_p)$, $T > \Theta_{III-IV}$, where $C = 2 \dots 4 \cdot 10^5 \text{ }^\circ\text{K}$ and $\Theta_p = 60 \dots 80 \text{ }^\circ\text{C}$.						54S3
c	Spontaneous polarization: $P_s \cong 12 \cdot 10^{-8} \text{ C m}^{-2} (\parallel c, \text{ in phase V})$. Coercive and critical field for normal and double hysteresis curve: Fig. 6.						55C2
9a	Birefringence: Fig. 7, 8.						
14a	Domain structure: See						55C2, 64p1, 62M9, 62W3
b	Dynamic properties: Fig. 9, 10.						

Tab. 1. NaNbO₃. Fractional coordinates x , y , z of atoms in unit cell at RT. [61W2]

	x	y	z
Na(1)	$\frac{1}{2}$	0.250	0
Na(2)	0.769	0.251	$\frac{1}{2}$
Nb	0.261	0.257	0.125
O(1)	$\frac{1}{2}$	0.208	0
O(2)	0.271	0.290	$\frac{1}{2}$
O(3)	0.010	0.532	0.121
O(4)	0.446	0.972	0.126

According to Ismailzade phase III consists of 4 phases (see Fig. 3). [63J4]
Transitions exhibit large temperature hysteresis, and the transition temperatures measured with decreasing temperature are given here.

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Tab. 2. NaNbO_3 . Lattice parameters at various temperatures. [56F1] and [54S3]

T [$^{\circ}\text{C}$]	Crystal symmetry	Lattice parameters	
		[56F1]	[54S3]
20	Monoclinic	$a' = c' = 3.914 \text{ \AA}$ $b' = 4 \cdot 3.881 \text{ \AA}$ $\beta' = 90^\circ 39'$	$a' = c' = 3.915 \text{ \AA}$ $b' = 4 \cdot 3.881 \text{ \AA}$ $\beta' = 90^\circ 40'$
390	Pseudotetragonal	$a = 2 \cdot 3.920 \text{ \AA}$ $c = 4 \cdot 3.926 \text{ \AA}$ $c/a = 2.0032$	$a = 2 \cdot 3.919 \text{ \AA}$ $c = 4 \cdot 3.927 \text{ \AA}$ $c/a = 2.0040$
420	Pseudotetragonal	$a = 2 \cdot 3.924 \text{ \AA}$ $c = 4 \cdot 3.924 \text{ \AA}$ $c/a \approx 2.0000$	$a = 2 \cdot 3.921 \text{ \AA}$ $c = 4 \cdot 3.927 \text{ \AA}$ $c/a = 2.0028$
560	Tetragonal (changing to simple perovskite-type cell)	$a = 2 \cdot 3.933 \text{ \AA}$ $c = 4 \cdot 3.940 \text{ \AA}$ $c/a = 2.0038$	— — —
640	Cubic	$a = 3.942 \text{ \AA}$	—

Tab. 3. NaNbO_3 . Lattice parameters of the subcell at various temperatures. [63I4]. See Fig. 3

T [$^{\circ}\text{C}$]	Subcell parameters				
	pseudomonoclinic I ($a' = c' > b'$, $\beta' > 90^\circ$)				
	a' [\AA]	b' [\AA]	$\beta' - 90^\circ$	a'/b'	V [\AA^3]
18 ... 20	3.914 ₇	3.885	40 ¹	1.0075 ₅	59.5 ₃
100	3.917	3.893 ₆	37	1.0060	59.7 ₄
150	3.919 ₅	3.898 ₇	33	1.0055	59.9
200	3.922 ₄	3.902 ₆	29	1.0050	60.0 ₅
250	3.924 ₃	3.907 ₅	26	1.0040	60.1 ₇
300	3.925 ₆	3.914	22	1.0030	60.3 ₂
340	3.926 ₃	3.917 ₅	18	1.0025	60.4
350	3.926 ₅	3.919	17	1.0020 ₂	60.4 ₂
	pseudomonoclinic II				
360	3.927 ₄	3.920	6	1.0020	60.45
380	3.927 ₈	3.921 ₃	5	1.0015 ₉	60.50
400	3.928 ₃	3.922 ₃	4	1.0015	60.5 ₂
	pseudomonoclinic III				
420	3.929 ₄	3.923	3	1.0015	60.5 ₅
440	3.930	3.924	3	1.0015	60.6 ₀
460	3.932	3.926 ₃	3	1.0015	60.70
	pseudomonoclinic IV				
480	3.933 ₅	3.927 ₅	3	1.0015 ₅	60.7 ₇
500	3.934 ₅	3.928 ₈	2	1.0015	60.8 ₂
510	3.935	3.929 ₅	2	1.0015	60.85
	tetragonal I				
T [$^{\circ}\text{C}$]	c [\AA]	$a = b$ [\AA]	c/a	V [\AA^3]	
520	3.936 ₇	3.929 ₅	1.0015 ₉	60.80	
540	3.938	3.930 ₂	1.0020	60.85	
560	3.939 ₈	3.931 ₆	1.0020 ₈	60.90	
	tetragonal II				
580	3.941 ₄	3.934 ₂	1.0020	61.00	
600	3.943 ₄	3.937 ₈	1.0015	61.15	
620	3.945 ₆	3.942	1.0010	61.30	
630	3.945	≈ 3.945	≈ 1.0000	61.40	
	cubic				
T [$^{\circ}\text{C}$]	a_0 [\AA]	V [\AA^3]	T [$^{\circ}\text{C}$]	a_0 [\AA]	V [\AA^3]
640	3.947 ₃	61.50	700	3.949 ₇	61.6 ₂
650	3.947 ₆	61.5 ₂	720	3.950 ₆	61.6 ₇
680	3.949	61.5 ₇			

Nr.

1a
b

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12

* Nu
** Fo

Nr. 1A-2 KNbO₃, Potassium niobate

1a b	Ferroelectricity in KNbO ₃ was first discovered by MATTHIAS in 1949. phase IV III II I state F F F P crystal system rhombohedral orthorhombic tetragonal cubic space group Bmm2 ^a -C _{2v} ¹⁴ Pm3m-O _b ¹ Θ -10 225 435 °C	49M4 *)63K2
	$P_s \parallel [001]$ in phase II (along [001] of phase I), $P_s \parallel [001]$ in phase III (along [110] of phase I), $P_s \parallel [111]$ in phase IV (along [111] of phase I). $T_{\text{mel}} = 1050^\circ\text{C}$ $\rho = 4.590 \cdot 10^3 \text{ kg m}^{-3}$ $a = 5.697 \text{ \AA}, b = 3.971 \text{ \AA}, c = 5.720 \text{ \AA}$ at RT. Transparent. Light yellow.	55R3, 58M3 52L1 67K4
2	Flux method (K_2CO_3 flux). Phase diagram of $\text{K}_2\text{CO}_3-\text{Nb}_2\text{O}_5$ system; see Pulling method from the $\text{K}_2\text{CO}_3-\text{Nb}_2\text{O}_5$ mixture Crystal form: square plate	51W1 55R3 58M3
3	Crystal structure: $Z = 1$ in phase I, II, IV. $Z = 2$ in phase III. Tab. 4, 5; Fig. 11.	
4	Temperature dependence of lattice parameters: Tab. 6; Fig. 12.	
5	Dielectric constant: Fig. 13, 14. $\chi = C/(T - \Theta_p)$, $T > \Theta_{\text{II}-\text{I}}$, where $C = 2.42 \cdot 10^5 \text{ K}$, $\Theta_p = 360^\circ\text{C}$. Nonlinear dielectric properties: $\xi = -1.62 \cdot 10^8 \text{ J C}^{-4} \text{ m}^5$, $\zeta = 1.79 \cdot 10^{10} \text{ J C}^{-6} \text{ m}^9$. Spontaneous polarization and coercive field: Fig. 15. $P_s = 26 \cdot 10^{-2} \text{ C m}^{-2}$ at $T = \Theta_p$.	56T3 56T3 56T3
6	Transition heat, transition entropy: Tab. 7.	56T3
7	Piezoelectricity: Fig. 16.	
12	NQR: Tab. 8; Fig. 17 ... 20.	

Tab. 4. KNbO₃. Atomic positions in fractional coordinates at RT in phase III. [67K4]

Nb	0, 0, 0
K	0, $\frac{1}{2}$, $\frac{1}{2} + z_K$
O(1)	0, $\frac{1}{2}$, z_1
O(2)	$\frac{1}{4} + x_2$, 0, $\frac{1}{4} + z_2$
z_K	+0.017
z_1	+0.021
z_2	+0.035
x_2	+0.004

Tab. 5. KNbO₃. Interatomic distances and bond angles at RT. [67K4]

	*	distance Å	**	*	angle °
Nb-O(1)	(2)	1.991 ± 0.001	O(2)(s)-Nb-O(2)(s)	(1)	97.4 ± 1.2
Nb-O(2)	(2)	1.863 ± 0.007	O(2)(l)-Nb-O(2)(l)	(1)	83.4 ± 1.0
Nb-O(2)	(2)	2.180 ± 0.009	O(2)(s)-Nb-O(2)(l)	(2)	89.7 ± 0.5
K-O(1)	(1)	2.837 ± 0.014	O(1)-Nb-O(2)(s)	(4)	92.3 ± 0.6
K-O(1)	(2)	2.848 ± 0.001	O(1)-Nb-O(2)(l)	(4)	87.5 ± 0.6
K-O(1)	(1)	2.883 ± 0.014	Nb-O(1)-Nb	(1)	172.8 ± 0.7
K-O(2)	(4)	2.792 ± 0.008	Nb-O(2)-Nb	(2)	168.6 ± 0.6
K-O(2)	(4)	2.873 ± 0.010			
O(1)-O(2)	(4)	2.780 ± 0.012			
O(1)-O(2)	(4)	2.884 ± 0.012			
O(2)-O(2)	(1)	2.802 ± 0.024			
O(2)-O(2)	(1)	2.894 ± 0.024			
O(2)-O(2)	(2)	2.860 ± 0.001			

* Numbers in this column indicate numbers of equal bonds or angles per formula unit.

* For the O-Nb-O angles, the letter s or l indicates whether the Nb-O(2) bond involved is short or long.

Tab. 6. KNbO₃. Lattice constants and volume of unit cell at various temperatures. [54S3]. a' , c' : lattice parameters of pseudotetragonal cell

T °C	$a' = c'$ Å	b Å	b/a	β	V Å ³
25	4.0375	3.9711	1.0167	90° 15'	64.73
125	4.0374	3.9797	1.0145	90° 15'	64.87
185	4.0363	3.9830	1.0134	90° 13'	64.89
205	4.0369	3.9839	1.0133	90° 14'	64.93
	$a = b$	c	c/a		
220	3.9972	4.0636	1.0166		64.92
230	3.9978	4.0640	1.0166		64.95
270	3.9992	4.0647	1.0164		65.01
320	4.0023	4.0639	1.0154		65.10
375	4.0048	4.0620	1.0143		65.15
410	4.0080	4.0567	1.0122		65.18
425	4.0214				65.03
450	4.0225				65.09
510	4.0252				65.22

Tab. 7. KNbO₃. Transition heat and transition entropy per mole. [54S1]

Transition	ΔQ_m cal mol ⁻¹	ΔS_m cal °K ⁻¹ mol ⁻¹
IV → III	32	0.12
III → II	85	0.17
II → I	190	0.28
	134	—

Tab. 8. KNbO₃. NQR spectrum. [54C1]. The measured frequency ratios intersect the calculated ratios in a straight line at constant $\eta = 0.806 \pm 0.002$.
 η = asymmetry parameter

Crystal structure	f MHz	Meas- ured ratio	Calculated ratio ($\eta = 0.806$)	Identifi- cation	$\epsilon^2 q Q/h$ MHz
orthorhombic (20 °C)	3.648	1.204	1.204	(9/2, 7/2)	23.120 ± 0.05
	3.030	1.198	1.196	(3/2, 1/2)	
	2.527	1.214	1.213	(7/2, 5/2)	
	2.085			(5/2, 3/2)	
rhombohedral (-196 °C)	2.674	($\eta = 0.0$)			
	2.004	1.335	1.333	(9/2, 7/2)	16.0 ± 0.1
	1.335	1.503	1.500	(7/2, 5/2)	
				(5/2, 3/2)	

Nr. 1A-3 NaTaO₃, Sodium tantalate

1a	It was reported by MATHIAS in 1949 that NaTaO ₃ is ferroelectric below 480 °C. No anomalies of the dielectric constants, however, were observed by SMOLENSKII et al.					49M1 57S3
b	phase	IV	III	II	I	
	state	(F)				
	crystal system	orthorhombic	orthorhombic	tetragonal	cubic	
	space group	Pc ₂ 1n-C _{2v}				
	Θ	480	550	630	°C	
	$a = 5.4941 \text{ \AA}$, $b = 7.7508 \text{ \AA}$, $c = 5.5130 \text{ \AA}$ at RT. The cubic cell in phase I becomes pseudomonoclinic in phase IV. Relation between the orthorhombic unit cell and the pseudomonoclinic cell: Fig. 21.					57K1 57K1 62I4 51V2
3	Crystal structure: $Z = 4$. Atomic positions: Tab. 9; Fig. 22.					
4	Temperature dependence of lattice parameters: Tab. 10; Fig. 23.					

Tab. 9. NaTaO₃. Fractional coordinates of atoms in the unit cell.
[57K1]

Na	$\left\{ \begin{array}{l} x: 0 - 0.01 \\ y: \frac{1}{4} + 0.03 \\ z: 0 + 0.02 \end{array} \right.$	$0 + 0.01$	$\frac{1}{2} - 0.01$	$\frac{1}{2} + 0.01$
Ta*	$\left\{ \begin{array}{l} x: \frac{1}{2} \\ y: 0 \\ z: 0 \end{array} \right.$	$\frac{1}{2}$	0	0
O(1)	$\left\{ \begin{array}{l} x: 0 - 0.02 \\ y: \frac{1}{4} + 0.01 \\ z: \frac{1}{2} + 0.02 \end{array} \right.$	$0 + 0.02$	$\frac{1}{2} + 0.02$	$\frac{1}{2} - 0.02$
O(2)	$\left\{ \begin{array}{l} x: \frac{1}{4} + 0.04 \\ y: 0 - 0.03 \\ z: \frac{1}{2} + 0.04 \end{array} \right.$	$\frac{1}{2} - 0.04$	$\frac{1}{4} - 0.04$	$\frac{3}{4} + 0.04$
O(3)	$\left\{ \begin{array}{l} x: \frac{1}{4} + 0.04 \\ y: \frac{1}{2} + 0.06 \\ z: \frac{1}{4} + 0.04 \end{array} \right.$	$\frac{1}{2} - 0.04$	$\frac{1}{4} - 0.04$	$\frac{3}{4} + 0.04$

Tab. 10. NaTaO₃. Temperature dependence of the pseudo-cell parameters. [62I4].
For the notations, see Fig. 21

T [°C]	23	100	200	300	400	450	480	500	550	580	600
$a' = c' [\text{\AA}]$	3.889 ₅	3.893 ₆	3.899 ₅	3.907	3.912 ₈	3.916	3.918	3.920	3.923	3.925 ₂	3.927
$b' [\text{\AA}]$	3.885 ₅	3.890 ₅	3.896 ₅	3.903 ₈	3.910 ₂	3.913 ₆	3.915 ₈	3.918	3.923	$\approx 3.925_8$	≈ 3.927
$\beta - 90^\circ$	22'00"	16'00"	9'00"	6'00"	4'00"	3'30"	2'00"	$\approx 2'00"$	1'30"	0'00"	0'00"
a'/b'	1.0010	1.0009	1.0009	1.0008	1.0006	1.0006	1.0005	1.0005	1.000	1.000	1.000
V [\AA^3]	58.8 ₀	59.0 ₀	59.2 ₅	59.5 ₅	59.8 ₅	60.0 ₀	60.1 ₀	60.2 ₀	60.3 ₅	60.4 ₅	60.5 ₅
T [°C]	630	660	680								
$b = a = c$ [\AA]	3.929	3.931	3.932 ₅								
V [\AA^3]	60.6 ₅	60.7 ₅	60.8 ₀								

Nr. 1A-4 KTaO₃, Potassium tantalate

1a	Ferroelectric activity was first reported by MATTHIAS in 1949; ^{a)} however, recent studies by WEMPLE have proved that the ferroelectric transition does not occur, at least above 1.6 °K. ^{b)}	^{a)} 49M1, 49M4 ^{b)} 64W2, 65W2
b	KTaO ₃ is cubic and its space group is Pm3m-O _b ¹ .	64W2, 65W2, 51V2 55R2, 56R2 58R1 51V2 64W2
	$T_{\text{melt}} = (1357 \pm 3)^\circ\text{C}$. $\rho = 6.97 \cdot 10^4 \text{ kg m}^{-3}$. $a = 3.9885 \text{ \AA}$ at RT. Transparent, colorless or pale blue (blue in oxygen-deficient crystals). Cleavage: along {100} planes. Hardness: nearly the same as quartz.	
2a	Flux method: KF flux, ^{a)} dark small crystals; K ₂ CO ₃ flux, ^{b)} large (≈ 10 mm) transparent crystals. Czochralski-Kyropoulos method: large (≈ 10 mm) good quality crystals.	^{a)} 62T5, 64W2 ^{b)} 66U1 64W2, 65W2, 67B7 66W8
	Floating technique: planar single crystals. Phase diagram of system K ₂ CO ₃ -Ta ₂ O ₅ : Fig. 24. Hydrothermal phase diagram K ₂ O-Ta ₂ O ₅ -H ₂ O at 400 °C:	67M2
3	$Z = 1$ Crystal structure: cubic perovskite type, (Pm3m-O _b ¹). K at 1a position; Ta at 1b position; O at 3c position.	51V1, 51V2

* All positions ± 0.002 .

Figuren S. 221ff.

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4	Nr. 1A-4 KTaO ₃ , continued $a = 3.9885 \text{ \AA at RT; } a = 4.0026 \text{ \AA at } 450^\circ\text{C.}$	51V2, 59B1	12a
5a	Dielectric constant at low frequencies: earlier studies showed a peak in the κ vs. T curve; ^{a)} recent measurements have shown that no peak exists down to 1.6°K. b) Fig. 25. $\kappa = 243$ at RT. $\kappa = \kappa_0 + C/(T - \Theta_p)$ $T > 30^\circ\text{K, where } \kappa_0 = 48, C = 5.7 \cdot 10^4 \text{ }^\circ\text{K, } \Theta_p = 4^\circ\text{K.}$ Loss tangent: $\tan \delta \approx 0.001$ at 200 kHz at RT. Dielectric constant in the GHz range: Fig. 26. Q values in the GHz range: $Q = 10^3 \dots 10^4.$ Dielectric loss in the far infrared frequency range: See 1A-4-9 below (Figs. 34, 35). Hydrostatic pressure dependence of the reciprocal dielectric constant: Fig. 27.	^{a)} 50H3 ^{b)} 65W2, 64W2 65W2 64W2 64R3 64W2	b
b	Effects of dc bias on κ at 4.2°K and at RT: Figs. 28, 29. Coefficients in free energy expansion: $\xi = 9 \cdot 10^9 \text{ V m}^5 \text{ C}^{-3}$ at $4.2^\circ\text{K}, \xi = (4 \pm 1) \cdot 10^9 \text{ V m}^5 \text{ C}^{-3}$ at 295°K.	65K1	13b
c	D vs. E curves show no hysteresis character down to 1.6°K. P vs. E at 4.2°K : see	65W2 64W2	
9a	Refractive index in visible region: Fig. 30. Reflectivity in far infrared region and the dispersion: Figs. 31, 32. Reflectivity data were used to obtain transverse optical modes of the lattice vibration by means of Kramers-Kronig relation (cf. Tab. 42). Transverse optical modes as a function of temperature: Tab. 11; Fig. 33. The square of the wave number $\tilde{\nu}_{11}$ for the "ferroelectric mode" is approximately linear to T : $\tilde{\nu}_{11}^2 \propto (T - \Theta_p)$. (Additional data are given on the ferroelectric soft mode, see 1A-4-13b). Effect of lattice vibration on the fluorescent spectrum of Eu ³⁺ in KTaO ₃ : see Imaginary part of the dielectric constant and the conductivity in the far infrared region: Figs. 34, 35. Absorption coefficient α depends on the degree of oxygen reduction in KTaO ₃ . Absorption coefficient near the interband absorption edge (about 3.6 eV) for insulating and semiconducting KTaO ₃ : Fig. 36 (for additional data, see Fig. 2 of reference). Absorption vs. wavelength of light: Fig. 37. Absorption vs. carrier concentration in semiconducting KTaO ₃ : Fig. 38. Optical absorption in impurity doped single crystals: for impurities Fe, Mn, Co and Cr, see	63M4, 67P4 67P4, 67F2 65S9 65W2 67B1 64W2 64G3, 63G3 67F4	17
b	Quadratic electrooptic constants ($6328 \text{ \AA, } 2 \dots 77^\circ\text{K.}$): $M_{11} - M_{12} = (0.16 \pm 0.01) \text{ m}^4 \text{ C}^{-2}; M_{44} = (0.12 \pm 0.01) \text{ m}^4 \text{ C}^{-2}.$ Electroreflectance and electroabsorption were studied using semiconducting KTaO ₃ . Effect of interface dc field on the reflectance of the (100) surface: Fig. 39. Electroreflectance spectra of (100) and (111) surfaces: Figs. 40, 41. Electroreflectance spectra of (100) and (111) surfaces: Figs. 40, 41. Effect of polarization of light on the electroreflectance: Fig. 42. Electroreflectance as a function of the surface polarization: Fig. 43. Electroreflectance singularities and the corresponding energies: Tab. 12. Electroabsorption near the absorption edge: Fig. 44. Fundamental absorption edge ($\approx 3.6 \text{ eV}$) shifts to higher energies with dc bias: Fig. 45.	67B1, 66B2 67F2 65S9	
d	Faraday rotation near the band edge: Fig. 46; Tab. 44.		
f	Electric-field-induced Raman effect: Fig. 47. (For the ferroelectric soft mode obtained from the Raman scattering, see Fig. 33). Fluorescence spectrum of Eu ³⁺ in KTaO ₃ : see		
10	Resistivity of insulating single crystal: $\rho > 10^8 \Omega \text{m}$ at RT. Most data on the transport properties have been obtained using oxygen-deficient semiconducting KTaO ₃ . Resistivity of oxygen-deficient single crystals as a function of temperature: Fig. 48. Hall mobility: $\mu_H = 3 \cdot 10^{-3} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}$ at RT (see also Tab. 13). $\mu_H \approx 8 \cdot 10^4 \text{ T}^{-3} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}, T > 100^\circ\text{K};$ Fig. 49. Hall coefficient and Hall mobility at 4.2°K and RT for several semiconducting KTaO ₃ : Tab. 13. Hall mobility vs. carrier concentration: Fig. 50. Scattering cross section vs. carrier concentration: see Ca concentration in doped KTaO ₃ vs. net ionized donor concentration: see Electrical conductivity vs. hydrostatic pressure: Fig. 51. Conductivity in the far infrared region: see Fig. 35. Seebeck coefficient: $Q = 550 \mu\text{V} \text{ }^\circ\text{K}^{-1}$ at RT. (Oxygen-deficient KTaO ₃ with $N = 3.5 \cdot 10^{23} \text{ m}^{-3}$). Effective mass estimated from the Seebeck coefficient: $m^* = (0.8 \pm 0.28) m_0$. Photoconductivity vs. $h\nu$ shows a peak at $h\nu = 3.58 \text{ eV.}$	65W2 65W2 66S17 66W5 65W2 65W2 65W2	

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31	12a	NMR of ^{181}Ta in KTaO_3 : spin-lattice relaxation time, $T_1 \approx 10^{-3}$ sec at RT; spin-spin relaxation time, $T_2 \approx 10^{-5}$ sec at RT; nuclear magnetic moment of ^{181}Ta ($J = 7/2$); $p_n = (2.340 \pm 0.001) \mu_n$ (uncorrected); $(p_n = (2.35 \pm 0.01) \mu_n$, after estimated corrections). Nuclear magnetic acoustic resonance: the absorption data were given for $\Delta m = \pm 2$ transition of ^{181}Ta as a function of the angle between magnetic field and sound axis [100].	60B2															
W2	b	ESR of Eu^{2+} and Gd^{3+} in KTaO_3 : Tab. 14. ESR of Fe^{3+} : $g = 1.99 \pm 0.01$; $ a = (345 \pm 10) \cdot 10^{-2} \text{ m}^{-1}$ at 4.2°K ; $a = (288 \pm 5) \cdot 10^{-2} \text{ m}^{-1}$ at RT (Fe^{3+} is on the Ta^{5+} site). $a = (30 \pm 1) \cdot 10^{-2} \text{ m}^{-1}$ at RT (Fe^{3+} is on the K^{1+} site). ESR Stark effect for Fe^{3+} : E_{bias} along [100] induces axial splitting term D ($D = 12 \cdot 10^{-2} \text{ m}^{-1}$ at $E_{\text{bias}} = 1.0 \text{ MV m}^{-1}$ at 4.2°K ; $D \propto E_{\text{bias}}$). ESR of Ni^{3+} located on Ta^{5+} site (low spin state) and on K^{1+} site: see ESR in Mn-doped, Co-doped and Cr-doped KTaO_3 : see	67M4 66U1 64W2 67H3 67H3 63W5, 64W2 67H3, 65H2 64W2															
57P4	13b	Phonon dispersion relation for the transverse optical branch: Fig. 52; Tab. 15. Temperature dependence of the ferroelectric soft mode: Fig. 53. The square of the phonon energy of the ferroelectric soft mode can be approximated by $(h\nu)^2 = 10^4 A/\chi$, $40^\circ\text{K} < T < 295^\circ\text{K}$; where $A = 2.825 (\text{meV})^2$, $\chi(T)$ is the dielectric constant. For the ferroelectric soft mode, see also 1A-4-9a. Phonon energies of the acoustic modes: Fig. 54.	67S11 67S11															
57F2	17	Etchant: single crystal is slowly etched by dilute HF. Band structure and the related properties: see references; also 1A-4-9a, 9b, 9d, 10, and Tab. 12. Band gap energies determined by various methods:	64W2 67F4, 67B1															
63G3		<table border="1"> <thead> <tr> <th>Method</th> <th>296 °K</th> <th>77 °K</th> </tr> </thead> <tbody> <tr> <td>Faraday rotation</td> <td>3.77 eV 3.62 eV</td> <td>3.79 eV 3.65 eV</td> </tr> <tr> <td>Electroreflectance singularities</td> <td>3.57 eV 3.80 eV</td> <td></td> </tr> <tr> <td>Absorption data</td> <td>3.75 eV</td> <td></td> </tr> <tr> <td>Energy at which $\alpha \approx 10^6 \text{ m}^{-1}$</td> <td>3.79 eV</td> <td></td> </tr> </tbody> </table> <p>Cyclotron resonance of semiconducting KTaO_3 at 70 GHz and 1.4°K: microwave skin depth, about $30 \mu\text{m}$; see reference paper for the microwave absorption vs. magnetic field curves.</p>	Method	296 °K	77 °K	Faraday rotation	3.77 eV 3.62 eV	3.79 eV 3.65 eV	Electroreflectance singularities	3.57 eV 3.80 eV		Absorption data	3.75 eV		Energy at which $\alpha \approx 10^6 \text{ m}^{-1}$	3.79 eV		67B1 65S13
Method	296 °K	77 °K																
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Energy at which $\alpha \approx 10^6 \text{ m}^{-1}$	3.79 eV																	

Tab. 11. KTaO_3 . Transverse optical modes at various temperatures [67P4]. The wave number $\tilde{\nu}_{t1}$ (ferroelectric soft mode) is temperature dependent.

$T [\text{°K}]$	$\tilde{\nu}_{t1}$	$\tilde{\nu}_{t2}$	$\tilde{\nu}_{t3}$
	$\cdot 10^2 \text{ m}^{-1}$		
12	25	196	—
126	58	198	551
232	79	198	551
295	88	199	550
463	106	199	—

Tab. 12. KTaO_3 . (Ca-doped). Singularities observed in electroreflectance spectra (in eV) [67F4]. See Figs. 40, 41

	E_1	E_2	A_1	A'_1	A_2
KTaO_3 (100)	3.57	3.80	4.40	4.88	5.50
KTaO_3 (111)	—	3.77	4.45	4.90	5.47
KTaO_3 (110)	3.55	3.80	4.47	4.85	5.50

Tab. 13. KTaO_3 (reduced). Hall coefficient R_H and Hall mobility μ_H at 295°K and 4.2°K for single crystals [65W2]. Carrier concentrations N are calculated from the 4.2°K Hall coefficient using $R_H = -1/Ne$

Sample Nr.	N_{calc} m^{-3}	R_H $\text{m}^3 \text{C}^{-1}$		μ_H $\text{m}^2 \text{V}^{-1} \text{sec}^{-1}$	
		(295°K)	(4.2°K)	(295°K)	(4.2°K)
1	$3.5 \cdot 10^{23}$	$20.3 \cdot 10^{-6}$	$18 \cdot 10^{-6}$	$2.7 \cdot 10^{-3}$	2.3
2	$6.0 \cdot 10^{23}$	$12.9 \cdot 10^{-6}$	$10.4 \cdot 10^{-6}$	$2.9 \cdot 10^{-3}$	1.9
3	$6.6 \cdot 10^{23}$	$11.5 \cdot 10^{-6}$	$9.4 \cdot 10^{-6}$	$3.1 \cdot 10^{-3}$	1.9
4	$2.4 \cdot 10^{24}$	$3.0 \cdot 10^{-6}$	$2.6 \cdot 10^{-6}$	$3.0 \cdot 10^{-3}$	1.1
5	$7.8 \cdot 10^{24}$	$1.0 \cdot 10^{-6}$	$0.80 \cdot 10^{-6}$	$3.0 \cdot 10^{-3}$	0.53
6	$1.3 \cdot 10^{25}$	$0.62 \cdot 10^{-6}$	$0.48 \cdot 10^{-6}$	$3.1 \cdot 10^{-3}$	0.34

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Figuren S. 227 ff.

Tab. 14. KTaO_3 . Parameters of ESR spectrum of Eu^{2+} and Gd^{3+} ions, doped in single crystals of KTaO_3 [66U1]

Para-magnetic center	Site	S	\mathcal{H}	ν GHz	T °K	g-factor	FS		HFS	
							b_{40}, b_{60} 10^{-2} m^{-1}	I	A 10^{-2} m^{-1}	
Eu^{2+}	K ⁺	7/2	(8)	9.1	77	1.990 ± 0.002	$b_{40} = (\pm) 16 \pm 2$	5/2	$ ^{151}\text{A} = 36 \pm 1$	
					4.2	1.990 ± 0.002	$b_{60} = (\pm) 1.2 \pm 0.6$	5/2	$ ^{153}\text{A} = 16 \pm 1$	
		7/2			77	1.990 ± 0.002	$b_{40} = -8.14 \pm 0.27$			
Gd^{3+}							$b_{60} = +0.47 \pm 0.3$			
							$b_{40} = -7.0 \pm 0.3$			
							$b_{60} = +0.5 \pm 0.5$			

Nr. 1A-5 CaTiO_3 , Calcium titanate (Perovskite)

Tab. 16. CaTiO_3 . Ion positions. [57K2]

4 Ti in 4(a):	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, 0; 0, \frac{1}{2}, \frac{1}{2}$
4 Ca in 4(c):	$x, \frac{1}{2}, z; \bar{x}, \frac{1}{2}, \bar{z}; \frac{1}{2} + x, \frac{1}{2}, \frac{1}{2} - z; \frac{1}{2} - x, \frac{1}{2}, \frac{1}{2} + z;$ with $x = 0, z = 0.030$.
4 O in 4(c):	with $x = \frac{1}{2} - 0.037, z = -0.018$.
8 O in 8(d):	$x, y, z; \frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} + z;$ $\bar{x}, \frac{1}{2} + y, \bar{z}; \frac{1}{2} + x, \bar{y}, \frac{1}{2} - z;$ $\bar{x}, \bar{y}, \bar{z}; \frac{1}{2} + x, \frac{1}{2} + y, \frac{1}{2} - z;$ $x, \frac{1}{2} - y, z; \frac{1}{2} - x, y, \frac{1}{2} + z;$ with $x = \frac{1}{2} - 0.018, y = -0.026, z = \frac{1}{2} - 0.018$.

Tab. 15. KTaO_3 . Phonon energies of the soft ferroelectric mode (transverse optical mode) at various temperatures [67S11]. The wave vector q at the zone boundary is 0.788 \AA^{-1} ($= \pi/a$). See Fig. 52

T °K	Phonon energy [meV] for $q [\text{\AA}^{-1}] =$		
	0	0.1	0.2
295	10.7	11.5	13.5
230	9.7		
170	8.6	10.0	12.5
120	7.3		
77	5.7	7.5	10.7
40	4.2	6.0	
28	3.6	5.9	10.5
15	3.0	5.3	
10	3.2	5.2	
4	3.1	5.3	9.8

1a	Specific heat anomaly associated with a phase transition was observed in CaTiO_3 at about 1260 °C by NAYLOR et al. in 1946. GRÄNICHER et al. reported that CaTiO_3 becomes cubic above 1260 °C.	46N1, 54G1
b	phase	II
	state	P
	crystal system	orthorhombic
	space group	Pcmn-D _{2h} ¹⁶
	Θ	$\approx 1260 \text{ }^{\circ}\text{C}$
	$\rho = 4.10 \cdot 10^3 \text{ kg m}^{-3}$ at RT.	
	$T_{\text{melt}} = 1960 \text{ }^{\circ}\text{C}$	
	$a = 5.3670 \text{ \AA}, b = 7.6438 \text{ \AA}, c = 5.4439 \text{ \AA}$ at RT. The ideal perovskite cubic unit cell becomes pseudo-monoclinic in phase II in the same manner as shown in Fig. 21. $\beta' = 90^\circ 48'$ at RT. Transparent, colorless.	
2	Flux method; flux: $\text{CaCl}_2, \text{BaCl}_2, \text{CaCl}_2 + \text{BaCl}_2, \text{Na}_2\text{CO}_3 + \text{K}_2\text{CO}_3$. Flame fusion method:	57K2 58L1, 62M3
3	Crystal structure: Z = 4 in phase II. Fig. 55; Tab. 16.	57K2
4	Lattice distortion: Fig. 56.	62M3
5a	Dielectric constant: $\kappa = 186, \tan \delta = 3 \cdot 10^{-4}$ at RT. Fig. 57.	46N1
6a	Specific heat: Fig. 58. Transition heat: $\Delta Q = 550 \text{ cal mol}^{-1}$ at $\Theta_{\text{II}-\text{I}}$.	62M3 57K2

9a	Nr. 1A-5 CaTiO_3 , continued Refractive indices: Fig. 59. Reflection and absorption: Fig. 60, 61.	
17	Hardness: Mohs 6.5 ... 7, Knoop 986	62M3
Nr. 1A-6 SrTiO_3, Strontium titanate		
1a	Ferroelectric-like behavior of SrTiO_3 was first observed by GRÄNICHER in 1956.	56G2
b	phase	II* I
state	(F)	P
crystal system	tetragonal	cubic**
space group		$\text{Pm}3\text{m}$ - O_h^1
Θ	110	°K
	$T_{\text{melt}} \approx 2000$ °C. $\rho = 5.11 \cdot 10^3$ kg m ⁻³ . $a = 3.905$ Å at RT. Transparent, colorless	63f2, 64l1 63f2 64L4
2a	Crystal growth: Flux method (flux: KF or 50% Na_2CO_3 + 50% K_2CO_3). Flame-fusion (Verneuil) method. Phase diagram of the system $\text{SrO}-\text{TiO}_2$ is given in Figs. 297 and 289 of [64l1].	57N1 61G1 64l1
3	Crystal structure: $Z = 1$. Fig. 62.	
4	Thermal expansion: Fig. 63.	
5a	Dielectric constant: Figs. 64 ... 76. Expression of κ vs. T curve: Curie-Weiss law: $\kappa = C/(T - \Theta_p)$, $T > 70$ °K, where $C = 7.83 \cdot 10^4$ °K, $\Theta_p = 28$ °K $\kappa = M/[(T_1/2) \coth(T_1/2 T) - T_0]$, $T < 50$ °K, where $T_0 = 38$ °K, $T_1 = 84$ °K, $M = 9 \cdot 10^4$ °K.	61M3 59W2, 62S2
b	Coefficients of free energy expansion at low temperatures:	66C6
c	Saturation polarization: Fig. 77. Remanent polarization: Fig. 78.	
d	Electrocaloric effect: Fig. 79. For additional data, see	64K5, 65H4, 61H1
6a	Specific heat: Fig. 80. Specific heat below 1 °K, see	61g1, 66A4
b	Thermal conductivity: Figs. 81, 82. For ceramics: see also	58Y1, 60Y1, 61g1, 66H9
7a	Piezoelectricity (dc bias induced piezoelectricity): Figs. 83, 84, 85.	
b	Electrostriction: Fig. 86.	
8a	Elastic compliances and stiffnesses: Tab. 17; Figs. 87, 88, 89.	
9a	Refractive indices: Tabs. 18, 19; Fig. 90. Reflectivity, absorption coefficient and dielectric constant: (i) Infrared region: Figs. 91 ... 95. See also Tab. 42. (ii) Visible and ultraviolet region: Figs. 96 ... 102. See also Tab. 43.	
b	Quadratic electrooptic effect: $M_{11} - M_{12} = (0.14 \pm 0.01) \text{ m}^4 \text{ C}^{-2}$ at 6328 Å (4.2 ... 300 °K).	64G3
c	Piezooptic effect: Tabs. 20, 21.	

* In phase II a hysteresis loop is observed, a), b) but the remanent polarization depends upon the amplitude of the applied field. According to LVRLE, phase II consists of three phases. a) [59W2], b) [61M3], [64L4]

** Generally the phase I is believed to be cubic but evidence of pseudo-cubic structure was reported by a few authors. [64L4], [66C6]

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Figuren S. 236ff.

9d	Nr. 1A-6 SrTiO ₃ , continued Faraday rotation: Fig. 103. See also Tab. 44.	67B1
e	Raman effect: Fig. 104. Brillouin scattering: Fig. 105. See	66K1 61g1 61g1
10	Electrical resistivity: $\rho > 10^7 \Omega\text{m}$ (good quality single crystal) at RT. Fig. 106. For additional data, see Tab. 22. Resistivity, Hall coefficient and Hall mobility of semiconductive samples: Tab. 23; Figs. 107 ... 110. For additional data, see Hall mobility for photo-excited electron: see Fig. 115. Piezoresistivity: Figs. 111, 112, 113. Photocconductivity: Figs. 114, 115. Photoemission: Fig. 116. Superconductivity: discovered in semiconductive SrTiO ₃ , by SCHOOLEY et al. in 1964. Figs. 117 ... 120. Tab. 24. Penetration depth of static magnetic field in superconductive SrTiO ₃ , is of the order of 10^{-5} m .	64F5, 67T6 66T10 64S5 66S16
11	Magnetic susceptibility: Tab. 25.	
12a	NMR: Fig. 121.	
b	ESR: Tab. 26; Figs. 122 ... 130.	
c	Mössbauer effect: Figs. 131, 132.	
13c	Inelastic neutron scattering: Tab. 27; Figs. 133, 134, 135.	
14a	Domain structure: A fine twin structure was observed in phase II. The appearance of the twin structure is similar to that of the 90° domains in tetragonal BaTiO ₃ . The dc field, however, does not change the twin structure.	61M3, 64L4
16	Radiation damage: Fig. 136.	
17	Etching and chemical polishing: Band structure and related properties: The band structure was determined theoretically by KAHN et al: Fig. 137. For discussions, see Magneto resistance, Shubnikov-deHaas effect. The conduction band consists of spheroids along [100] having 3 minima at X_s . The transverse and longitudinal effective electron mass: $m_t = 1.5 m_0 (\pm 15\%)$, $m_l = 6.0 m_0 (\pm 30\%)$.	66R6 64K1 65S18 66F3, 67F3 67F3

Tab. 17. SrTiO₃. Elastic constants at RT

s_{11}	s_{12}	s_{13}	c_{11}	c_{12}	c_{13}	Method	Note	Reference
$10^{-12} \text{ m}^2 \text{ N}^{-1}$			10^{11} N m^{-2}					
3.3	-0.74	8.4	3.48	1.01	1.19	composite-bar pulse	c calculated from s	58p5
3.729	-0.909	8.091	3.181	1.025	1.236	pulse	s calculated from c	63B2
3.772	-0.926	8.233	3.156	1.027	1.215		s calculated from c	63W1
± 0.023	± 0.010	± 0.040	± 0.027	± 0.027	± 0.006			

Tab. 18. SrTiO₃. n vs. λ at 21 °C. [57G1]

λ Å	n	λ Å	n	λ Å	n
4200	2.6050	5400	2.4386	6600	2.3771
4300	2.5810	5500	2.4312	6700	2.3737
4400	2.5585	5600	2.4245	6800	2.3703
4500	2.5394	5700	2.4182	6900	2.3674
4600	2.5236	5800	2.4122	7000	2.3645
4700	2.5101	5900	2.4069	7100	2.3617
4800	2.4970	6000	2.4019	7200	2.3590
4900	2.4846	6100	2.3971	7300	2.3564
5000	2.4734	6200	2.3928	7400	2.3535
5100	2.4636	6300	2.3886	7500	2.3514
5200	2.4548	6400	2.3846	7600	2.3490
5300	2.4464	6500	2.3807	7700	2.3468

Tab. 19. SrTiO₃. n vs. λ [65B9]

λ μm	n	λ μm	n
0.45	2.537	1.8	2.270
0.5	2.472	2.0	2.264
0.6	2.402	2.2	2.258
0.7	2.363	2.4	2.2524
0.8	2.340	2.6	2.2490
0.9	2.326	2.8	2.2395
1.0	2.315	3.0	2.2315
1.1	2.306	3.2	2.2236
1.2	2.299	3.4	2.2143
1.4	2.287	3.6	2.2058
1.6	2.279	3.8	2.1951

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Tab. 20. SrTiO_3 . Π_{66} vs. λ at $(27 \pm 1)^\circ\text{C}$. [57G1]

λ Å	Π_{66} $10^{-13} \text{ m}^2 \text{ N}^{-1}$	λ Å	Π_{66} $10^{-13} \text{ m}^2 \text{ N}^{-1}$
4200	-3.69	6000	-4.92
4300	-3.74	6100	-4.99
4400	-3.78	6200	-5.05
4500	-3.99	6300	-5.12
4600	-3.965	6400	-5.13
4700	-4.13	6500	-5.18
4800	-4.09	6600	-5.22
4900	-4.22	6700	-5.29
5000	-4.33	6800	-5.52
5100	-4.32	6900	-5.48
5200	-4.41	7000	-5.55
5300	-4.51	7100	-5.62
5400	-4.59	7200	-5.77
5500	-4.575	7300	-5.73
5600	-4.62	7400	-5.78
5700	-4.69	7500	-5.79
5800	-4.79	7600	-5.825
5900	-4.85	7700	-5.98

Tab. 21. SrTiO_3 . $\Pi_{21} - \Pi_{11}$ vs. λ at $(27 \pm 1)^\circ\text{C}$. [57G1]

λ Å	$\Pi_{21} - \Pi_{11}$ $10^{-13} \text{ m}^2 \text{ N}^{-1}$	λ Å	$\Pi_{21} - \Pi_{11}$ $10^{-13} \text{ m}^2 \text{ N}^{-1}$
4200	9.03	6000	9.95
4300	9.23	6100	9.94
4400	9.03	6200	9.91
4500	9.26	6300	9.84
4600	9.12	6400	9.82
4700	9.12	6500	9.88
4800	9.14	6600	9.96
4900	9.16	6700	9.92
5000	9.35	6800	9.98
5100	9.44	6900	9.99
5200	9.61	7000	9.91
5300	9.54	7100	9.92
5400	9.68	7200	9.94
5500	9.56	7300	9.99
5600	9.85	7400	10.05
5700	9.85	7500	9.90
5800	9.86	7600	9.92
5900	9.88	7700	10.02

Tab. 22. SrTiO_3 (single crystal). Effects of electrode material on the apparent conductivity [65C6]. Measurements were made by the two terminal method at $T = 130^\circ\text{C}$, $t = 24$ hours after the application of the field $E = 100 \text{ kV m}^{-1}$

Electrode material	$\sigma [\Omega^{-1} \text{ m}^{-1}]$ after 24 h at 130°C	Form of σ vs. t curve	
		After 24 h	After 24 h
Au	$4.8 \cdot 10^{-7}$	Fall then rise	
Ag	$8.8 \cdot 10^{-8}$	As for gold	
Sn	$8.8 \cdot 10^{-9}$	Fall followed by slow rise but without saturation	
Cr	$6.0 \cdot 10^{-11}$	Continuous fall tending toward steady value	
Cd	$9.5 \cdot 10^{-11}$	Similar to chromium	
Al	$2.9 \cdot 10^{-10}$	Similar to chromium (for a field of 400 kV m^{-1} behavior is like that of gold)	

Tab. 23. SrTiO_3 (single crystal). The 300°K and 2°K Hall coefficient R_H and Hall mobility μ_H values and the 300°K electron concentrations for semiconductive single crystals. [67T6]. In the first column, (Nb) means Nb-doped samples, the other samples are reduced ones

Sample	300 °K		2 °K		$n = \frac{1}{eR_H(300^\circ\text{K})} \text{ m}^{-3}$
	R_H $10^{-6} \text{ m}^3 \text{ C}^{-1}$	μ_H $10^{-4} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}$	R_H $10^{-6} \text{ m}^3 \text{ C}^{-1}$	μ_H $10^{-1} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}$	
5	0.26	6.5	0.25	1.0	$2.4 \cdot 10^{25}$
2	0.62	5.2	0.77	1.8	$1.0 \cdot 10^{25}$
3	1.8	7.2	3.9	2.7	$3.5 \cdot 10^{24}$
6	5.3	8.0	11.0	3.1	$1.2 \cdot 10^{24}$
12	14.0	8.0			$4.5 \cdot 10^{23}$
9	23.0	5.8			$2.7 \cdot 10^{23}$
13(Nb)	0.22	5.5	0.22	3.3	$2.8 \cdot 10^{25}$
8(Nb)	0.58	4.8	0.63	8.2	$1.1 \cdot 10^{25}$
10(Nb)	3.4	6.2	3.3	12.0	$1.8 \cdot 10^{24}$
14(Nb)	14.0	6.7	11.0	13.0	$4.5 \cdot 10^{23}$
15(Nb)	22.0	5.4	18.0	19.0	$2.8 \cdot 10^{23}$
11(Nb)	44.0	6.0	33.0	22.0	$1.4 \cdot 10^{23}$

Tab. 24 see page 50

Tab. 25. $\Delta \chi_{\text{mag}}$: Susceptibility in pure and reduced single crystals [66F2].
 χ_{mag} represents the contribution from the charge carriers; $\Delta \chi_{\text{mag}}$ is obtained by measuring the
 χ_{mag} of reduced crystals and subtracting the "pure" diamagnetic and Van Vleck contributions.
 N = carrier concentration; T_{deg} = degeneracy temperature; m^* = density-of-state effective mass

Sample	N at 4.2 °K m ⁻³	T_{deg} °K	χ_{mag} or $\Delta \chi_{\text{mag}}$ · 10^{-7} cm ³ g ⁻¹			m^* at 4.2 °K [m ₀]
			300 °K	78 °K	4.2 °K	
pure	—	—	χ	-1.02	-0.92	—
28 h, 950 °C hydrogen	$6 \cdot 10^{24}$	28	$\Delta \chi_1$	$+0.037$	$+0.073$	—
5 h, 1200 °C hydrogen (carbon boat)	$7.5 \cdot 10^{25}$	148	$\Delta \chi_2$	$+0.270$	$+0.523$	5.1
reoxidized 18 h, 700 °C, air	—	—	χ	-1.016	-1.012	—
27 h, 1370 °C hydrogen (carbon boat)	$5.3 \cdot 10^{26}$	550	$\Delta \chi_3$	$+1.704$	$+1.763$	4.9

^{a)} [62B2] ^{b)} [62S12]

Tab. 26. SrTiO₃. Summary of the properties of ESR spectrum in SrTiO₃ for various doped paramagnetic ions

Para-magnetic center	Site	S	\mathcal{H}	GHz	T °K	g-factor		FS	HFS	Ref.	Literature
						g_{\parallel}	g_{\perp}				
Cr ³⁺	Ti ⁴⁺	3/2	(5)	9	80	1.9788 ± 0.007	(isotropic)	$D = 2 \pm 0.3,$ $E = 0$	$\mathfrak{n}A = 0$	3/2	^{a)} 58M7
					300	1.9780 ± 0.007	(isotropic)	$D = 0,$ $E = 0$	$\mathfrak{n}A = 16.2 \pm 0.3$		^{f)} 62M6
Mn ⁴⁺	Ti ⁴⁺	3/2	(5)	10	77	1.994 ± 0.001	(isotropic)	$D = +1.0,$ $E = 0$	$\mathfrak{n}A = -69.4 \pm 1$		^{g)} 59M4
Fe ³⁺	Ti ⁴⁺	5/2	(7)	9	1.9	2.004 ± 0.001	(isotropic)	$D = -0.7,$ $E = 0$	$\mathfrak{n}A = -69.4 \pm 1$		
					4.2	2.004 ± 0.001	(isotropic)	$D = +17.9 \pm 1.0,$ $E = 0$			^{a)} 59D2
					77	2.004 ± 0.001	(isotropic)	$D = +16.1 \pm 0.7,$ $E = 0$			^{b)} 58M8
					300	2.004 ± 0.001	(isotropic)	$D = +7.3 \pm 0.3,$ $E = 0$			^{c)} 58M8
Ni ³⁺	Ti ⁴⁺	1	(4)	10	80	2.204 ± 0.001	(isotropic)	$D = 1.0,$ $E = -197.7 \pm 0.7$			^{d)} 62R3
Ni ¹⁺ or Ni ³⁺	Ti ⁴⁺	1/2	(2)	10	80	2.029 ± 0.001	2.352 ± 0.001				^{e)} 62R3
					203						

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Para-magnetic center	Site	S	\mathcal{H}	GHz	T °K	g-factor		FS	HFS	Ref.	Literature
						g_{\parallel}	g_{\perp}				
Landolt-Bornstein						$D, E, \alpha [10^{-2} \text{ m}^{-1}]$	$I \cdot \mathfrak{n}A_{\text{av}} [10^{-2} \text{ m}^{-1}]$				

Para-magnetic center		Site	S	ν GHz	T o K	ϵ -factor		FS		HFS		Ref.	Literature
Ni ²⁺	Ti ⁴⁺					ϵ_{\parallel}	ϵ_{\perp}	D, E, α [10^{-2} m^{-1}]	I [$\mu A_{\parallel}, \mu A_{\perp} [10^{-2} \text{ m}^{-1}]$]				
Ni ²⁺ or Ni ³⁺	Ti ⁴⁺	1/2	(2)	10	4.2	2.110 ± 0.002	2.213 ± 0.002					e)	62R3
				20	2.136 ± 0.001	2.202 ± 0.001							
				80	2.172 ± 0.001	2.184 ± 0.001							
				203	(isotropic)	2.180 ± 0.002						e)	62R3
Ce ³⁺	—	1/2	(2)	10	4.2	3.005 ± 0.005	1.118 ± 0.003					e)	62R3
		—	1/2	(2)	10	4.2	2.609 ± 0.003	2.472 ± 0.003				e)	62R2
				16	2	2.61 ± 0.01	2.470 ± 0.005						
				35	2	2.62 ± 0.01	2.470 ± 0.005						
Yb ³⁺	—	1/2	(3)	16	2	2.11 ± 0.01	2.780 ± 0.005						62R2
				35	2	2.10 ± 0.005							
				16	50	2.18 ± 0.01	2.720 ± 0.005						
				35	50	2.17 ± 0.005	2.720 ± 0.005						
				35	65	(2.25)	2.70 ± 0.01						
								FS [10^{-2} m^{-1}]					
								b_{20}	b_{40}	b_{60}			
Eu ²⁺	—	7/2	(8)	16	2	1.99 ± 0.001	-10 ± 4	106.6 ± 2	6.7 ± 2	$5/2$	$ \frac{\mu A_{\parallel}}{\mu A_{\perp}} = 36.2$	62R2	
				300	2	1.99 ± 0.001	0	105.9 ± 2	1.1 ± 2	$5/2$	$ \frac{\mu A_{\parallel}}{\mu A_{\perp}} = 17.6$	f)	
Gd ³⁺	Sr ²⁺	7/2	(8)	16	2	1.992 ± 0.002	-362.5 ± 0.5	-3.2 ± 0.5	1.4 ± 0.5				62R2
		12, 18		4.2	4.2	1.992 ± 0.002	-362.5 ± 0.5	-3.24 ± 0.5	1.4 ± 0.5				62R1
				77	77	1.992 ± 0.002	-233.6 ± 0.5	-4.8 ± 0.5	-0.25 ± 0.5				b)
				300	300	1.992 ± 0.002		-5.7 ± 0.2	0.5 ± 0.3				

- a) $\xi = [100], \eta = [010], \zeta = [001].$
b) Deviations from spin Hamiltonian (7) is ascribed to a covalent bonding by MÜLLER. However, AISENBERG et al. find a negligible contribution of the covalent bonding. [59A1].
c) Spectrum is due to a double quantum absorption between $S_z = -1$ and $S_z = +1$ levels.
d) At least fifteen inequivalent sites are observed.
e) Three inequivalent spectra are observed with axes parallel to the cubic [100], [010] and [001].
f) Effects of temperature and pressure on Cr³⁺, Fe²⁺, Eu²⁺, and Gd³⁺ spectra. [64R2].
g) Fe²⁺ spectra due to nearest charge compensation. [64K7].
h) Electric field dependence of Gd³⁺ spectra. [66S3].

Tab. 24. SrTiO_3 (ceramics containing Ba or Ca in mol%). Superconductive properties of $(\text{Ba}_x\text{Sr}_{1-x})\text{TiO}_3$ and $(\text{Ca}_x\text{Sr}_{1-x})\text{TiO}_3$ [67S8]. H_{c1} is the point at which the magnetization curve first deviates from linearity; $H_{c1}(0)$ is the extrapolated value for $T \rightarrow 0^\circ\text{K}$.
 N = Carrier concentration Θ_c = superconducting transition temperature

% Ba or Ca	N 10^{25} m^{-3}	Θ_c $^\circ\text{K}$	$H_{c1}(0)$ Oe	% Ba or Ca	N 10^{25} m^{-3}	Θ_c $^\circ\text{K}$	$H_{c1}(0)$ Oe
—	2.7	0.18		10.0	4.2	0.25	
—	5.8	0.30	2.8	12.5	4.5	<0.10	
—	6.4	0.25	2.8	2.5 (Ca)	5.0	0.32	
—	1.7	0.10		5.0	9.2	0.30	
—	12.0	0.17		7.5	74.0	<0.06	
—	23.0	0.10		7.5	8.7	0.43	
2.5 (Ba)	6.0	0.52		7.5	0.2	<0.06	(3.5) ^{a)}
2.5	0.3	0.23		7.5	0.6	0.37	
5.0	6.7	0.50	3.9	7.5	2.0	0.48	
7.5	7.0	0.29		7.5	9.3	0.39	
7.5	0.05	0.22		10.0	13.0	0.29	
7.5	34.0	0.09		20.0	6.7	0.50	
7.5	0.5	0.25		30.0	0.6	<0.05	
7.5	2.3	0.27		30.0	1.9		
7.5	15.0	0.45					

Nr. 1A-7 CdTiO_3 , Cadmium titanate

1a	CdTiO_3 was reported by SMOLENSKII in 1950 to be ferroelectric below $50 \dots 60^\circ\text{K}$. In 1950 HULM et al. denied its ferroelectricity but HEGENBARTH supported SMOLENSKII's findings.	50S7, 50H2, 59H4
b	phase II I state (F) ^{a)} crystal system orthorhombic ^{b)} space group $\text{Pc}2_1\text{n}^b\text{-C}_{2v}^a$	^{a)} 50S7 ^{b)} 57K1
	Θ_c $-223 \dots -213^\circ\text{C}$ Lattice constants: $a = 5.348 \text{ \AA}$, $b = 7.615 \text{ \AA}$, $c = 5.417 \text{ \AA}$ at RT. The relation between the orthorhombic unit cell and the pseudo-cubic monoclinic cell is the same as in the case of NaTaO_3 ; see Fig. 21.	50S7 57K1
2	Flux method (flux: 40 wt% NaCl + 40 wt% NaBO_2 + 20 wt% Na_2CO_3).	57K1
3	$Z = 4$. Crystal structure in phase I: Tab. 28; Fig. 138.	
5a	Dielectric constant: $\kappa = 250$ at RT. $\kappa = C/(T - \Theta_p)$, $C = 4.5 \cdot 10^4 \text{ }^\circ\text{K}$.	50S7, 50H2
b	Effect of E_{bias} on κ : Fig. 139.	

			Positions				Estimated error
			x:	y:	z:		
	Cd		$0 + 0.006$	$0 - 0.006$	$\frac{1}{2} + 0.006$	$\frac{1}{2} - 0.006$	± 0.002
			$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	
			$0 + 0.016$	$0 - 0.016$	$\frac{1}{2} - 0.016$	$\frac{1}{2} + 0.016$	± 0.002
	Ti		$\frac{1}{2} + 0.005$	$\frac{1}{2} - 0.005$	$0 + 0.005$	$0 - 0.005$	± 0.005
			0	$\frac{1}{2}$	$\frac{1}{2}$	0	
			$0 - 0.065$	$0 + 0.065$	$\frac{1}{2} + 0.065$	$\frac{1}{2} - 0.065$	± 0.010
	O(1)		$0 - 0.03$	$0 + 0.03$	$\frac{1}{2} + 0.03$	$\frac{1}{2} - 0.03$	± 0.015
			$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	
			$\frac{1}{2} + 0.05$	$\frac{1}{2} - 0.05$	$0 + 0.05$	$0 - 0.05$	± 0.025
	O(2)		$0 - 0.03$	$0 - 0.03$	$\frac{1}{2} - 0.03$	$\frac{1}{2} - 0.03$	± 0.015
			$\frac{1}{2} + 0.06$	$\frac{1}{2} + 0.06$	$\frac{1}{2} - 0.06$	$\frac{1}{2} - 0.06$	± 0.015
	O(3)		$\frac{1}{2} + 0.05$	$\frac{1}{2} - 0.05$	$\frac{1}{2} - 0.05$	$\frac{1}{2} + 0.05$	± 0.005
			$\frac{1}{2} + 0.07$	$\frac{1}{2} + 0.07$	$0 + 0.07$	$0 + 0.07$	± 0.015
			$\frac{1}{2} + 0.06$	$\frac{1}{2} + 0.06$	$\frac{1}{2} - 0.06$	$\frac{1}{2} - 0.06$	± 0.015

^{a)} This specimen is not spherical, so that the value of $H_{c1}(0)$ quoted is only approximate.

^{b)} Hall coefficient appeared to be affected by magnetic history of specimen at liquid helium temperature.

Nr. 1A-8 BaTiO₃, Barium titanate

(Responsible authors for this section are as follows: IKEDA, NAKAMURA, NOMURA, SAWAGUCHI, SHIOZAKI and TOYODA, abbreviated as INAnoSAShiTō).

1a	The anomalous dielectric properties of BaTiO ₃ were discovered on ceramic specimens independently by WAINER and SOLOMON in 1942, by OGAWA in 1944 and by WUL in 1945. The ferroelectric activity of BaTiO ₃ was reported independently by von HIPPEL and co-workers in 1944 and by WUL in 1946. The structural change associated with the cubic-tetragonal phase transition was observed, by means of x-rays, by MEGAW in 1945, independently of the above dielectric studies.						42W1, 44O1, 45W1 44V2 46W2 45M1																														
b	<table border="1"> <thead> <tr> <th>phase</th><th>IV^{a)}</th><th>III^{a)}</th><th>II^{b)}</th><th>I^{b)}</th><th></th></tr> <tr> <th>state</th><th>F^{a)}</th><th>F^{a)}</th><th>F^{c)}</th><th>P^{b)}</th><th></th></tr> </thead> <tbody> <tr> <td>crystal system</td><td>rhombo-hedral^{a)}</td><td>ortho-rhombic^{a)}</td><td>tetragonal^{b)}</td><td>cubic^{b)}</td><td>hexagonal^{d)*}</td></tr> <tr> <td>space group</td><td>R3m-C_{3v}^{a)}</td><td>Amm2-C_{2v}^{a)}</td><td>P4mm-C_{4v}^{b)}</td><td>Pm3m-O_h^{b)}</td><td>C63/mmc-D_{6h}^{d)}</td></tr> <tr> <td>Θ</td><td>-90^{a)}</td><td>5^{a)}</td><td>120^{b)}**</td><td>1460^{d)}</td><td>°C</td></tr> </tbody> </table>						phase	IV ^{a)}	III ^{a)}	II ^{b)}	I ^{b)}		state	F ^{a)}	F ^{a)}	F ^{c)}	P ^{b)}		crystal system	rhombo-hedral ^{a)}	ortho-rhombic ^{a)}	tetragonal ^{b)}	cubic ^{b)}	hexagonal ^{d)*}	space group	R3m-C _{3v} ^{a)}	Amm2-C _{2v} ^{a)}	P4mm-C _{4v} ^{b)}	Pm3m-O _h ^{b)}	C63/mmc-D _{6h} ^{d)}	Θ	-90 ^{a)}	5 ^{a)}	120 ^{b)} **	1460 ^{d)}	°C	^{a)} 49K2, 49R1 ^{b)} 45M1 ^{c)} 46V1, 46W1 ^{d)} 55R1
phase	IV ^{a)}	III ^{a)}	II ^{b)}	I ^{b)}																																	
state	F ^{a)}	F ^{a)}	F ^{c)}	P ^{b)}																																	
crystal system	rhombo-hedral ^{a)}	ortho-rhombic ^{a)}	tetragonal ^{b)}	cubic ^{b)}	hexagonal ^{d)*}																																
space group	R3m-C _{3v} ^{a)}	Amm2-C _{2v} ^{a)}	P4mm-C _{4v} ^{b)}	Pm3m-O _h ^{b)}	C63/mmc-D _{6h} ^{d)}																																
Θ	-90 ^{a)}	5 ^{a)}	120 ^{b)} **	1460 ^{d)}	°C																																
	$P_s \parallel [001]$ in phase II (along [100] of phase I). $P_s \parallel [001]$ in phase III (along [110] of phase I). $P_s \parallel [111]$ in phase IV (along [111] of phase I). The directions of P_s are illustrated along with lattice distortions in Fig. 140. $T_{\text{melt}} = 1618$ °C. Tetragonal form (phase II): $\rho = 6.02 \cdot 10^3$ kg m ⁻³ (calculated from lattice constants) $a = 3.9920$ Å, $c = 4.0361$ Å at 20 °C. Transparent, light brown. Hexagonal form: $a_{\text{hex}} = 5.735$ Å, $c_{\text{hex}} = 14.05$ Å at RT. $\rho = (6.1 \pm 0.1) \cdot 10^3$ kg m ⁻³ .						51W2 51R1 48B3																														
2a	Crystal growth: Flux method (flux KF ^{a)} or TiO ₂ -rich melt ^{b)}). Pulling method (top-seeded solution growth technique using excess TiO ₂ as the solvent). Melting method (with limited success). Tab. 29; Fig. 141.						^{a)} 54R1, ^{b)} 65S8																														
b	Crystal forms: For butterfly-type: Fig. 142. For chunky type: Fig. 143. For hexagonal form: Fig. 144.						63L3 50V2																														
3	Crystal structure of phase I: $Z = 1$. Tab. 30. Crystal structure of phase II: $Z = 1$. Tab. 31. Crystal structure of phase III: $Z = 2$. Tab. 32; Fig. 145, 146; Tab. 33. Crystal structure of phase IV: $Z = 1$. Crystal structure of hexagonal form: $Z = 6$. Tab. 34, 35; Fig. 147.																																				
4	Lattice constants of phase I, II, III, and IV: Phase I: $a = 3.996$ Å at 120 °C. Phase II: $a = 3.9920$ Å, $c = 4.0361$ Å at 20 °C. Phase III: $a = 3.990$ Å, $b = 5.669$ Å, $c = 5.682$ Å at -10 °C. Phase IV: $a = 4.001$ Å, $\alpha = 89^\circ 51'$ at -168 °C. Thermal expansion: Fig. 148, 149; Tab. 36, 37; Fig. 150. Lattice distortion due to p : Fig. 151.						47M3 51R1 57S2 57J2																														
5a	Dielectric constant: Fig. 152, 153, 154, 192. Dielectric dispersion: Fig. 155 ... 159. Further data from optical measurements: Fig. 201; Tab. 42. Effect of p on ϵ : Fig. 160, 161, 162. Phase diagram in regard to p : Fig. 163, 164. Effect of E_{bias} on Θ_f : $d\Theta_f/dE_{\text{bias}} = 1.43 \cdot 10^{-5}$ °K V ⁻¹ m; on ϵ : Fig. 165.						53M2																														
b	Non-linear dielectric properties: Fig. 166. $\xi = -5.5 \cdot 10^8$ J C ⁻⁴ m ⁶ , $\zeta = 1.7 \cdot 10^{10}$ J C ⁻⁶ m ⁹ .						53M2																														

* The transition from the hexagonal form to the cubic one is very sluggish and the hexagonal form can be produced by rapid cooling from above 1460 °C.

In most papers this Curie point has been reported to be about 120°C , but it seems to be about 130°C for pure BaTiO₃ [65J2].

			14a
5c	Nr. 1A-8 BaTiO ₃ , continued Spontaneous polarization: Fig. 167, 168, 169. Coercive field: Fig. 170, 171, 172. Effect of p on P_s : Fig. 173.		
d	Electrocaloric effect: Fig. 174. Pyroelectricity: Fig. 175.		
6a	Specific heat: Fig. 176, 177. Transition heat, transition entropy: Tab. 38.		
b	Thermal conductivity: Fig. 178, 179.		
7a	Piezoelectricity: Tab. 39, 40; Fig. 180 ... 183.		
b	Electrostriction: Fig. 184, 185.		
8a	Elastic compliances and stiffnesses: Tab. 41. See also Tab. 40. Fig. 186 ... 193.		
b	Non-linear elastic properties: Fig. 194.		
9a	Refractive indices: Fig. 195, 196, 197. Birefringence: Fig. 198, 199. Reflection and absorption: (i) Far-infrared region, Fig. 200, 201; Tab. 42. (ii) Infrared region, Fig. 202, 203, 204. (iii) Visible region, Fig. 205, 206, 207. (iv) Ultraviolet region, Fig. 208; Tab. 43; Fig. 209, 210, 211. For the effect of E_{bias} on the absorption edge, see	67G1	
b	Linear electrooptic effect: Fig. 212 ... 215. Quadratic electrooptic effect: $(M_{11} - M_{12}) = (+ 0.13 \pm 0.02) \text{ m}^4 \text{ C}^{-2}$ at 408 ... 433 °K, measured at 6328 Å.	64G3	
d	Faraday rotation: Fig. 216; Tab. 44.		
e	Non-linear optical properties: Susceptibility for SHG (second harmonic generation) (relative values, see Sec. IC): $d_{15} = 35 \pm 3$, $d_{31} = 37 \pm 3$, $d_{33} = 14 \pm 1$, determined with the Nd-doped CaWO ₄ laser beam. Fig. 217.	64M2	
f	Raman scattering: Fig. 218.		
g	Luminescence: Fig. 219, 220.		
10	Conductivity of as-grown crystals and ceramics: The data vary from sample to sample depending on the purity and the method of preparation: only representative data are given here. Fig. 221 ... 225. Conductivity associated with doping or reduction (including PTC (Positive Temperature Coefficient) or resistivity: $d\varrho/dT > 0$): Fig. 226 ... 230. Reference papers on PTC anomaly: Tab. 45. Piezoresistivity: Fig. 231, 232. For additional data, see Breakdown strength: Fig. 233, 234. For additional data, see	59S1, 63M1, 67G4	
	Photoconductivity and photoemission: Fig. 235, 236. Other transport properties: In <i>n</i> -type single-domain crystals, the electron mobility is anisotropic at RT; $\mu_{\perp c} \approx 1.2 \cdot 10^{-4} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}$, and $\mu_c \approx 0.13 \cdot 10^{-4} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}$ at 26 °C. In <i>n</i> -type single-domain crystals, the energy separation ($\Delta u = 10^{-2} \dots 10^{-1} \text{ eV}$) between the <i>c</i> -axis conduction band minima and the <i>a</i> -axis conduction band minima has been estimated vs. T . In <i>n</i> -type single-domain crystals, the density-of-state mass $m^* = (6.5 \pm 2) m_0$. Data are available on the Hall coefficient and conductivity of single domain crystals having donor concentrations of $N = 8.5 \cdot 10^{24} \text{ m}^{-3}$ and of $N = 2.5 \cdot 10^{23} \text{ m}^{-3}$. Fig. 237. Seebeck-effect: Fig. 238.	58I3, 59F1, 64K3, 64U1 67B2 67B2 67B2 67B2	
12b	ESR: Tab. 46; Fig. 239 ... 243.		0.0
c	Mössbauer effect: Fig. 244 ... 247.		0.0
13b	Diffuse X-ray scattering: Fig. 248, 249, 250. Inelastic neutron scattering: Fig. 251.		0.0 0.0 0.0 0.0 The O(2)

14a	Domain structure: Domains have been observed by various methods: polarized light ^a), X-rays ^b), electron microscope ^c), etching method ^d), powder pattern method ^e), and decoration method ^f). Fig. 252 ... 255.	^{a)} 48M1, ^{a)} 49F1, 52M3 ^{b)} 63B13, ^{b)} 64N1, 65C3, ^{b)} 64L1 ^{c)} 62T1, 63B9, ^{c)} 67R4, 64T2, ^{c)} 66R5, 67R2 ^{d)} 55H2 ^{e)} 59P1 ^{f)} 66S8
b	Domain wall motion: Domain wall motion has been observed optically ^a) and by repeated differential etching. ^b) The domain shapes in motion depend on the applied field and temperature. ^c) Fig. 256. The wall velocity is proportional to $\exp(-\delta/E)$ at relatively low field. δ = activation field for domain wall motion. Fig. 257 ... 267.	^{a)} 59M2, 60S2 ^{b)} 63S13 ^{c)} 63S13 58M4, 59M3
15	Surface layer: The first suggestion about the existence of surface layers of BaTiO ₃ crystals was made by KÄNZIG ^a) on the basis of electron diffraction studies of very small particles of BaTiO ₃ ^b). The dependence of the following quantities on the thickness of the crystals has been observed as evidence of the existence of surface layers: domain wall velocity ^c), dielectric constant ^d), optical absorption coefficient ^e) and electroluminescence spectra ^f). Pyroelectric current was observed above the Curie point and discussed in connection with surface layers ^g). A few models of surface layers have been proposed ^h). According to TANAKA and HONJŌ ⁱ), the surface layer, if it exists, seems to be very thin.	^{a)} 55K1 ^{b)} 54A1 ^{c)} 56M4, 61M2, 65C1 ^{d)} 61S4, 62C3 ^{e)} 60C3 ^{f)} 58H1, 65B7, 66B6 ^{g)} 56C1 ^{h)} 56M4, 61F2, 59D3, 65C1 ⁱ⁾ 64T2
16	Radiation damage: Fig. 268, 269.	
17	Energy band structure: Fig. 270.	

Tab. 29. BaTiO₃. Solubility in KF solution. [54K1]

T	1000	1050	1100	1150	1200	1250	1300	°C
BaTiO ₃	4	6	9	12.5	17	22.5	28.5	mole %

Tab. 30. BaTiO₃. Fractional coordinates of atoms in the unit cell of phase I. [52M2]

	x	y	z
Ba	0	0	0
Ti	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
O	$\frac{1}{2}$	$\frac{1}{2}$	0
	$\frac{1}{2}$	0	$\frac{1}{2}$
	0	$\frac{1}{2}$	$\frac{1}{2}$

Tab. 31. BaTiO₃. Shift of atoms in fractional coordinates of phase II from the positions of phase I. [51K1], [55F1], [61E3]

δz_{Ti}	$\delta z_{\text{O}(1)}$	$\delta z_{\text{O}(2)}$	Ba B_{11} B_{33}	Ti B_{11} B_{33}	O(1) B_{11} B_{22}	O(2) B_{11} B_{22} B_{33}	References
0.014	-0.032	0	0.48	0.13	0.13	0.48	51K1
0.014	-0.023	-0.014	0.273	0.152	0.334	0.267	55F1
0.015	-0.024	-0.020	0.27 0.28	0.53 0.21	0.90 0.08	0.60 0.49 0.07	61E3
0.012	-0.026	0	0.27 0.28	0.46 0.30	0.90 0.50	0.60 0.90 0.90	61E3

The positions of atoms in the unit cell are Ba at (0, 0, 0), Ti at ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2} + \delta z_{\text{Ti}}$), O(1) at ($\frac{1}{2}$, $\frac{1}{2}$, $\delta z_{\text{O}(1)}$) and O(2) at ($\frac{1}{2}$, 0, $\frac{1}{2} + \delta z_{\text{O}(2)}$).

Tab. 32. BaTiO_3 . Fractional coordinates of atoms in the unit cell of phase III. [57S2]

	x	y	z
Ba	0	0	0
	0	$\frac{1}{2}$	$\frac{1}{2}$
Ti	$\frac{1}{2}$	0	$\frac{1}{2} + \delta z_{\text{Ti}}$
	$\frac{1}{2}$	$\frac{1}{2}$	δz_{Ti}
O(1)	0	0	$\frac{1}{2} + \delta z_{\text{O}(1)}$
	0	$\frac{1}{2}$	$\delta z_{\text{O}(1)}$
O(2)	$\frac{1}{2}$	$\frac{1}{2} + \delta y_{\text{O}(2)}$	$\frac{1}{2} + \delta z_{\text{O}(2)}$
	$\frac{1}{2}$	$\frac{1}{2} + \delta y_{\text{O}(2)}$	$\frac{1}{2} + \delta z_{\text{O}(2)}$
	$\frac{1}{2}$	$\frac{1}{2} - \delta y_{\text{O}(2)}$	$\frac{1}{2} + \delta z_{\text{O}(2)}$
	$\frac{1}{2}$	$\frac{1}{2} - \delta y_{\text{O}(2)}$	$\frac{1}{2} + \delta z_{\text{O}(2)}$

$$\delta z_{\text{Ti}} = +0.010; \delta z_{\text{O}(1)} = -0.010; \delta z_{\text{O}(2)} = -0.013; \delta y_{\text{O}(2)} = +0.003.$$

Tab. 34. BaTiO_3 . Fractional coordinates of atoms in the unit cell of hexagonal structure. [48B3]

$$\begin{aligned} & 2\text{Ba}(1) \text{ at } (\bar{b}), & \\ & 4\text{Ba}(2) \text{ at } (\bar{f}), & z = 0.097, \\ & 2\text{Ti}(1) \text{ at } (\bar{a}), & \\ & 4\text{Ti}(2) \text{ at } (\bar{f}), & z = 0.845, \\ & 6\text{O}(1) \text{ at } (\bar{h}), & x = 0.522, \\ & 12\text{O}(2) \text{ at } (\bar{k}), & x = 0.836, z = 0.076 \end{aligned}$$

Tab. 35. BaTiO_3 . Interatomic distances of hexagonal structure. [48B3] in the Ti_2O_9 group

$\text{O}(1) - \text{O}(1)$	$= 2.49 \text{ \AA}$	in the shared face.
	$= 3.25 \text{ \AA}$	in the same layer but the atoms do not belong to the same shared face.
$\text{O}(2) - \text{O}(2)$	$= 2.91 \text{ \AA}$	
$\text{O}(1) - \text{O}(2)$	$= 2.91 \text{ \AA}$	
$\text{Ti}(2) - \text{O}(1)$	$= 1.96 \text{ \AA}$	
$\text{Ti}(2) - \text{O}(2)$	$= 2.02 \text{ \AA}$	
in the TiO_6 octahedra		
$\text{O}(2) - \text{O}(2)$	$= 2.82 \text{ \AA}$	in the same layer.
$\text{O}(2) - \text{O}(2)$	$= 2.69 \text{ \AA}$	
$\text{Ti}(1) - \text{O}(2)$	$= 1.95 \text{ \AA}$	between adjacent layers.

Tab. 36. BaTiO_3 . Lattice constants and unit cell volume at various T . [51R1]

T °C	a Å	b Å	c Å	V Å ³
+ 20	3.9920	3.9920	4.0361	64.317
+ 4	3.9910	3.9911	4.0357	64.282
$\Theta_{\text{III}-\text{II}}$				
+ 4	4.0185	3.9860	4.0162	64.319
- 99	4.0170	3.9750	4.0150	64.093
$\Theta_{\text{IV}-\text{III}}$				
- 99	4.0015	4.0015	4.0020	64.079
- 160	3.9996	3.9996	3.9997	63.981

Accuracy of measurement below RT was $\pm 0.0007 \text{ \AA}$.

Tab. 33. BaTiO_3 . Comparison of atomic shifts in phase III and phase II with respect to different origins. The coordinate of atoms of [55F1] and [57S2] are used for phase II and III, respectively. [57S2]

	Orthorhombic	Tetragonal
δz	Ti O(1) O(2)	Ba at (000)
		$+0.06 \text{ \AA}$
		-0.06 \AA
		-0.07 \AA
$\delta y_{\text{O}(2)}$		$\pm 0.02 \text{ \AA}$
		-
		Origin is chosen to give $\delta z_{\text{O}(2)} = 0$
δz	Ti Ba O(1)	$+0.13 \text{ \AA}$
		$+0.07 \text{ \AA}$
		$+0.02 \text{ \AA}$
		$+0.15 \text{ \AA}$
		$+0.09 \text{ \AA}$
		-0.03 \AA

Tab. 37. BaTiO_3 . Linear thermal expansion coefficients along a , b , and c axes. [51R1]

T °C	α_a $10^{-6} \text{ }^{\circ}\text{C}^{-1}$	α_b $10^{-6} \text{ }^{\circ}\text{C}^{-1}$	α_c $10^{-6} \text{ }^{\circ}\text{C}^{-1}$
+ 20	15.7	15.7	6.2
+ 4	4.9	28.4	-0.9
- 99	7.8	7.8	8.2
- 160			

Tab. 38. BaTiO_3 . Transition heats and transition entropies

Transition	ΔQ_m cal mol ⁻¹	ΔS_m cal mol ⁻¹ °K ⁻¹	References
IV \rightarrow III	8 \pm 2	0.04	52S5
	14.3	0.07	52V1
	12	0.06	52T1
III \rightarrow II	22 \pm 4	0.076	52S5
	15.5	0.054	52V1
	16	0.058	52T1
II \rightarrow I	50 \pm 5	0.125	52S5
	47	0.12	52V1
	47	0.12	48B1

Tab. 41. BaTiO₃ (single crystal and ceramics). Elastic constants. [66b1]

	s_{11}^E	s_{11}^D	s_{33}^E	s_{33}^D	s_{13}^E	s_{13}^D	s_{12}^E	s_{12}^D	s_{34}^E	s_{34}^D	s_{66}	T	References
10 ⁻¹² m ² N ⁻¹													
single crystal	9.26 11.2	7.25 8.05	15.7 8.18	10.8 9.5	-2.35 -2.61	-3.15 -2.98	-5.24 -2.85	-3.26 -1.95	18.4 23.3	12.4 18.3	8.84 22.3	25 25	50C2 51B1 58B2
ceramics	8.55 9.1	8.7 9.5	8.93 7.1	6.76 7.1	-2.7 -2.7	-2.9 -2.9	-1.9 -1.9	-1.9 -2.8	17.5 22.8	17.5 23.6	23.6 23.6	25 25	56B3 64b1
	c_{11}^E	c_{11}^D	c_{33}^E	c_{33}^D	c_{13}^E	c_{13}^D	c_{34}^E	c_{34}^D	c_{44}^E	c_{44}^D	c_{66}		
single crystal	275.1	282.6	164.9	178.1	179.0	186.5	151.6	141.6	54.34	80.64	113.1	25	66b1, 58B2
ceramics	166 150 165.6	168 150	162 146	189 171 180.7	76.6 68	78.2 66	77.5 66	71.0 57	42.9 44	54.6 57	44.8 43	25 25	56B3 64b1 55H5

Tab. 42 ... 45 see page 58

Tab. 46. BaTiO₃. Summary of the ESR parameters for various paramagnetic centers in doped BaTiO₃.

Paramagnetic center	Site	S	ν	GHz	T	g-factor	FS		HFS		Ref.	Literature	
							D, E, a, F [10 ⁻² m ⁻¹]	I	A, B [10 ⁻² m ⁻¹]	I			
Mn ²⁺	Ti ⁴⁺	5/2	(7)	9.3	78	2.0016 ± 0.0005	$D = 56 \pm 5$		$\frac{5}{2}$	$\frac{\text{ss}A_{ }}{\text{ss}A_{\perp}} = \frac{\text{ss}A_{ }}{\text{ss}A_{\perp}} = 79.8 \pm 0.5$	60I1		
							2.0023 ± 0.0005	$D = 65 \pm 5$		$\frac{\text{ss}A_{ }}{\text{ss}A_{\perp}} = 78.6 \pm 0.5$			
Ba ²⁺		5/2	(7)	9.3	RT	2.0009 ± 0.001	$a = 14 \pm 5$			$\frac{\text{ss}A_{ }}{\text{ss}A_{\perp}} = 79 \pm 0.5$	63O1		
						2.0002 ± 0.001	$D = +(\frac{215}{16.76} \pm \frac{2}{0.94})$	$E = 0$		$\frac{\text{ss}A_{ }}{\text{ss}A_{\perp}} = -(\frac{77.4}{82.3} \pm \frac{0.6}{0.8})$			
						438	2.002 ± 0.001	$D = 0$	$a = +(12.11 \pm 0.94)$	$E = 0$	$\frac{\text{ss}A_{ }}{\text{ss}A_{\perp}} = -(\frac{79.3}{79.3} \pm 0.4)$		

Dat.	ν_{\perp}	ν_{\parallel}			$D = 0$	$E = 0$	$\frac{\text{ss}A_{\parallel}}{\text{ss}A_{\parallel}} = - (79.3 \pm 0.4)$	$\frac{\text{ss}A_{\perp}}{\text{ss}A_{\parallel}} = - (12.11 \pm 0.94)$

Para-magnetic center	Site	S	\mathcal{K}	GHz	T_K	g-factor	FS		Ref.	Literature			
							D, E, a, F, b [10^{-2} m^{-1}]	I					
Fe ³⁺	Ti ⁴⁺	5/2	(7)	5 ... 7.5,	393,	2.003	$D = 0$		d) e) f)	59H ⁵ , 62R ¹ , 63S ²)			
				10, 16.3	433		$a = 102 \pm 12$						
				300	2.0036 \pm 0.002		$D = +929$	$E = 0$					
				276	2.0036 \pm 0.002		$a = +91 \pm 20$						
				213	2.0036 \pm 0.002		$D = -530 \pm 10$						
		7/2	(3)		$a = +105 \pm 20$		$a = +105 \pm 20$		g)	64S ³) ^a)			
				77	2.0036 \pm 0.002		$D = -640 \pm 10$						
				173	2.003 \pm 0.002		$E = 0 \pm 1.3$						
							$a = 0 \pm 10$						
							$a = +115 \pm 10$						
Co ²⁺	Ti ⁴⁺	1/2	(3)	9	4	4.347 (isotropic)	$D = -23 \pm 5$		h)	67Z2			
							$a - F = +113 \pm 10$						
Gd ³⁺	Ba ²⁺	7/2	(8)	12, 18	300	1.995 \pm 0.003	b_{20}	b_{40}	i)	62R1			
				425	RT	1.995 \pm 0.003	-	b_{60}					
Ti ⁴⁺		10				-293.6 \pm 1.0	$+4.0 \pm 1.0$	1.6 ± 1.0	j)	64T1			
				436		-	-	≈ 6					
Fe ³⁺	Ti ⁴⁺	10	(3)			-	24 ± 0.9	-3.7 ± 2.8	k)	66T3			
							23.3 ± 0.4	-1.8 ± 0.4					
Electron	oxygen vacancy	1/2	(2)	10	55	g_{\parallel}	g_{\perp}		l)	66S21, 66T2, 67T3			
						1.950 \pm 0.005	2.459 \pm 0.003						
						78	1.935 \pm 0.005	2.51 ± 0.02	m)	63S12			
								1.911					

a) Temperature dependence of D^* in the tetragonal phase is linear. [65V4].

b) Forbidden transition lines ($\Delta M = \pm 1, \Delta m = \pm 1$) are observed. [63O], [64J5].

c) Temperature dependence of $\text{ss}A$. [67Z1].

d) Fe³⁺ spectra are studied with a d.c. bias electric field near transition temperature from cubic to tetragonal phase and from tetragonal to orthorhombic phase. [63S3].

e) Forbidden transition lines ($\Delta M = 2, 3, 4, 5$) are observed in the rhombohedral phase. [64S3].

f) Fe³⁺ spectra due to the oxygen vacancy; $g_{\parallel} \approx 2$, $g_{\perp} = 6.0 \pm 0.1$ at 77 K. [65G1].

g) Hyperfine structure of an electron captured by an oxygen vacancy. [64D1].

h) Mn²⁺ ion takes the place of Ti⁴⁺ lattice site in ceramics, while it takes the place of Ba²⁺ in a single crystal.

i) Positive a is assumed.

j) Fe³⁺ spectra in a single-domain specimen.

Figuren S. 259ff.

II 1 Oxide des Perowskit-Typs

Tab. 42. BaTiO_3 , SrTiO_3 , TiO_2 , KTaO_3 . Dispersion parameters calculated from the Kramers-Kronig analysis [62S11]. See Fig. 201

	$\kappa' = \kappa_\infty + \sum_i 4\pi \rho_i \nu^2 \frac{\nu_i^2 - \nu^2}{(\nu_i^2 - \nu^2)^2 + \gamma_i^2 \nu^2}$	$\kappa'' = \sum_i 4\pi \rho_i \nu_i^2 \frac{\nu_i \nu}{(\nu_i^2 - \nu^2)^2 + \gamma_i^2 \nu^2}$		
	BaTiO_3 Ordinary ray	SrTiO_3	TiO_2 Ordinary ray	KTaO_3
$\lambda_1; \nu_1$	20.4; 491	18.4; 544	20.0; 500	18.2 ± 0.2 ; 549 ± 6
γ_1/ν_1	0.059 ± 0.002	0.049 ± 0.002	0.044 ± 0.004	0.043 ± 0.009
$4\pi \rho_1$	0.60 ± 0.03	1.56 ± 0.06	2.0 ± 0.2	2.4 ± 0.5
$\lambda_2; \nu_2$	54.8; 183	56.3 ± 0.5 ; 178 ± 2.0	25.8; 388	49.8; 200.8
γ_2/ν_2	0.030 ± 0.006	0.039 ± 0.004	0.058 ± 0.006	0.055 ± 0.011
$4\pi \rho_2$	2.2 ± 0.4	3.6 ± 0.4	1.08 ± 0.1	7.6 ± 1.5
$\lambda_3; \nu_3$	296 ± 8 ; 33.8 ± 0.9	114.3 ± 1.1 ; 87.7 ± 0.9	54.8 ± 0.5 ; 183 ± 1.8	107.5 ± 2.0 ; 93.0 ± 2.0
γ_3/ν_3	2.5 ± 0.1	0.5 ± 0.1	0.19 ± 0.01	0.5 ± 0.1
$4\pi \rho_3$	1830 ± 70	311 ± 62	81.5 ± 4.1	163 ± 33

Resonance wavelength λ_i in 10^{-6} m; resonance frequency ν_i in 10^2 m $^{-1}$; width γ_i ; strength $4\pi \rho_i$.

Tab. 43. BaTiO_3 , SrTiO_3 , TiO_2 . Energies of fundamental absorption edges (in eV) at RT. [65C2]

	E_0	A_1	A_2	A_3	B_1	B_2	C_1	C_2	D	E	
SrTiO_3	3.2	4.00	4.86	5.5	6.52	7.4	9.2	9.9	12.5	15.3	eV
BaTiO_3	3.2	3.91	4.85		6.10	7.25	10.3	11.8	12.8	15	eV
TiO_2 ($E \perp c$)	3.97	5.52			6.50	7.64	8.53	9.24	11	14.1	eV

Tab. 44. BaTiO_3 , SrTiO_3 , KTaO_3 , $\text{KTA}_{0.35} \text{Nb}_{0.65} \text{O}_3$ (KTN), TiO_2 . Band gap energies $\hbar \omega_g$ (in eV). [67B1]. See Fig. 46, 103, 216, 430. F_1 , F_2 : different dispersion functions $F_i(\omega/\omega_g)$, see [67B1]

	SrTiO_3		BaTiO_3	KTAO_3		KTN	TiO_2	
	296 °K	77 °K	403 °K	296 °K	77 °K	296 °K	296 °K	
Faraday rotation $\hbar \omega_g$ for F_1	3.40	3.43	3.25	3.77	3.79	3.54	3.62	eV
Faraday rotation $\hbar \omega_g$ for F_2	3.21	3.26	3.11	3.62	3.65	3.36	3.37	eV
Energy of reflectivity peak or shoulder	3.20	—	3.20	—	—	3.70	—	eV
Energy of electroreflectance singularity	—	—	3.20	3.57	—	3.60	3.00	eV
$\hbar \omega_g$ from absorption data	3.40	—	—	3.80	—	—	3.30	eV
Energy at which absorption coefficient $\alpha \approx 10^4 \text{ cm}^{-1}$	3.37	—	3.26	3.75	—	3.45	3.18	eV

Tab. 45. BaTiO_3 (reduced or doped). List of reference papers on PTC anomaly

Materials (dopants)	References	Materials (dopants)	References
Single crystal BaTiO_3 : reduced	57H1, 63K3, 64I4, 64G4, 65M1, 65U2 64B11	Ceramics BaTiO_3 BaTiO_3 : La	63H5, 65U2 59S1, 63T3, 64J1, 65M1
BaTiO_3 : Nb		BaTiO_3 : Ce BaTiO_3 : Sm BaTiO_3 : Gd BaTiO_3 : Sb (Ba-Sr) TiO_3 (Ba-Sr) TiO_3 : La BaTiO_3 : Sr, Ce, Sn BaTiO_3 : Sr, Ca, Sn BaTiO_3 : Sr, Bi BaTiO_3 : Mg, Ce BaTiO_3 : Zr, Ce BaTiO_3 : Si, Ce	63T3 63G5 65U2 65A3 61H5, 65A3 59S1, 61T1, 63T3 61S1 61S1 63T3 61S1 61S1 61S1

Nr. 1A-	F Si pl st cr sp Θ a 2a C b 3 C P 4 T L 5a D a1 C 6a S Δ Δ c T 7a P 9a B L F 12b E 14a D 16 F
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Nr. 1A-9 PbTiO₃, Lead titanate

1a	Ferroelectric activity was reported independently by SHIRANE et al. and by SMOLENSKII in 1950.				50S4 50S6
b	phase	III ^{b)*}	II ^{a)}	I ^{a)}	^{a)51S6} ^{b)55K3} ^{c)46M2}
	state		F ^{a)}	P ^{a)}	
	crystal system		tetragonal ^{c)}	cubic ^{a)}	
	space group		P4mm-C _{4v} ¹	Pm3m-O _h ¹	
	Θ	-100 ^{b)}	490 ^{a)}	°C	
		$a = 3.904_5 \text{ \AA}$	$c = 4.152_4 \text{ \AA}$ at RT (in phase II).		46M2
2a	Crystal growth: KF flux method; PbCl ₂ flux method. Crystal form: Fig. 271.				58K1, 52N2
3	Crystal structure: Positional parameters: Tab. 47, 48. Projection of crystal structure: Fig. 272, 273.				
4	Thermal expansion: Fig. 274 ... 280. Dependence of lattice parameters on hydrostatic pressure: Fig. 281.				
5a	Dielectric constants: Fig. 282. Small dielectric anomaly was observed at about -100 and -150 °C. Curie-Weiss constant: $C = 1.1 \cdot 10^5 \text{ ^\circ K}$ (single crystal).				56K2 62B4
6a	Specific heat: Fig. 283.				
		II-I			
	ΔQ_m	1150	cal mol ⁻¹		51S7
	ΔS_m	1.6	cal °K ⁻¹ mol ⁻¹		51S7
c	Thermal conductivity: Fig. 284.				
7a	Piezoelectric properties: Tab. 49.				
9a	Birefringence: Fig. 285. Infrared absorption: Fig. 286, 287. Frequencies of infrared modes: Tab. 50.				
12b	ESR: Tab. 51.				
14a	Domain structures were observed by polarized light.				52N2, 58K1, 59K1
16	Radiation damage: Fig. 288.				

Tab. 47. PbTiO₃. Positional parameters of atoms at RT. [56S5]

	x	y	z
Pb	0	0	0
Ti	$\frac{1}{2}$	$\frac{1}{2}$	0.540
O(1)	$\frac{1}{2}$	$\frac{1}{2}$	0.112
O(2)	$\frac{1}{2}$	0	0.612
	0	$\frac{1}{2}$	0.612

Tab. 48. PbTiO₃. Bond lengths in Å at RT (phase II) and at 490 °C (phase I) [56S5]. O(1)+ represents the O(1) ion closer to Ti, O(1)- that further away from Ti. Similarly O(2)+ is closer to Pb

phase	II (at RT)	I (at 490 °C)
Ti-O(1)+	1.78	1.89
Ti-O(1)-	2.38	
Ti-O(2)	1.98	
Pb-O(1)	2.80	2.80
Pb-O(2)+	2.53	
Pb-O(2)-	3.20	

* Phase transition II-III was reported to occur only if the cooling rate is extremely slow. [55K3]

Tab. 49. PbTiO_3 (modified ceramics). Electromechanical constants at RT. [68U1]

Additive	$\text{PbNb}_{4/8}\text{O}_3$ 5.0 mol%	$\text{BiZn}_{1/2}\text{Ti}_{1/2}\text{O}_3$ 5.0 mol%	$\text{Bi}_{2/3}\text{Zn}_{1/3}\text{Nb}_{2/3}\text{O}_3$ 5.0 mol%	
a	3.915	3.904	3.911	Å
c	4.104	4.148	4.133	Å
c/a	1.049	1.062	1.057	
ϱ	7.19	7.68	7.12	10^3 kg m^{-3}
porosity	0.105	0.036	0.10	
Θ	466	524	494	°C
$\tilde{\nu}_1$	—	195	244	
$\tilde{\nu}_3$	226	147	203	
d_{31}	10	3.9	7.4	$10^{-12} \text{ C N}^{-1}$
d_{33}	37	37	47	$10^{-12} \text{ C N}^{-1}$
g_{31}	5.2	3.0	4.1	$10^{-3} \text{ m}^2 \text{ C}^{-1}$
g_{33}	16	28	28	$10^{-3} \text{ m}^2 \text{ C}^{-1}$
s_{11}^E	1.2	1.2	1.1	$10^{-11} \text{ m}^2 \text{ N}^{-1}$
s_{33}^E	1.1	0.95	1.1	$10^{-11} \text{ m}^2 \text{ N}^{-1}$
Q_{mech} for s_{11}	336	54	326	
for s_{33}	71	74	76	
k_{15}	—	0.40	0.36	
k_{31}	0.068	0.031	0.052	
k_{33}	0.23	0.32	0.35	

Tab. 50. PbTiO_3 . Wave numbers in 10^2 m^{-1} and symmetries of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

	$\tilde{\nu}_1$ (Ti-O stretch)	$\tilde{\nu}_2$ (Ti-O ₃ torsion)	$\tilde{\nu}_3$ (O-Ti-O bend)	$\tilde{\nu}_4$ (cation-TiO ₃ lattice mode)
	530 (E_u, A_1)	400 (B_1, E_u)	220 (E_u, A_1) 172	83 (E_u, A_1)

Tab. 51. PbTiO_3 . g-factors at RT. [64G1]

Paramagnetic center	Site	S	\mathcal{H}	ν GHz	T °K	g-factor	
						g_{\parallel}	g_{\perp}
Fe ³⁺	Ti ⁴⁺	1/2*	(2)	8.8	RT	2.009 ± 0.005	5.97 ± 0.02

The spectrum up to 300 °C and down to -120 °C did not show any fundamental change.

Nr. 1A-10 CaZrO₃, Calcium zirconate

1	A few physical properties of CaZrO ₃ were studied in comparison with those of some perovskite-type ferroelectrics. The crystal was reported to be orthorhombic with the cell dimensions $a = 5.587 \text{ \AA}$, $b = 8.008 \text{ \AA}$, $c = 5.758 \text{ \AA}$ at RT.	55C1
4	Linear thermal expansion: $\alpha = 8.55 \cdot 10^{-6} \text{ }^{\circ}\text{C}^{-1}$ between 23 °C and 223 °C; $\alpha = 9.53 \cdot 10^{-6} \text{ }^{\circ}\text{C}^{-1}$ between 223 °C and 333 °C for ceramics of bulk density $\varrho = 4.95 \cdot 10^3 \text{ kg m}^{-3}$	65B10
9	Infrared absorption: Fig. 289, 290; Tab. 52.	

Tab. 52. CaZrO₃. Wave numbers in 10^2 m^{-1} and symmetry of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

	$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O ₃ torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO ₃ lattice mode)
	515 (B_1, B_2, A_1) (377) (418)	340 (B_1, B_2, A_2) (377) (418)	228 (B_1, B_2, A_1) 186	153 (B_1, B_2, A_1) 96

* The fictitious spin is $\frac{1}{2}$ [64G1].

Nr. 1A-11 SrZrO₃, Strontium zirconate

1	A few physical properties of SrZrO ₃ were studied in comparison with those of some perovskite-type ferroelectrics. The crystal was reported to be pseudo-cubic with $a' = 4.099 \text{ \AA}$ at RT.	57R2
4	Linear thermal expansion: $\alpha = 8.75 \cdot 10^{-6} \text{ ^\circ C}^{-1}$ between $23 \text{ }^\circ\text{C}$ and $320 \text{ }^\circ\text{C}$; $\alpha = 9.34 \cdot 10^{-6} \text{ ^\circ C}^{-1}$ between $320 \text{ }^\circ\text{C}$ and $700 \text{ }^\circ\text{C}$ for ceramics of bulk density $\rho = 5.00 \cdot 10^3 \text{ kg m}^{-3}$.	65B10
9	Infrared absorption: Fig. 291, 292; Tab. 53.	

Tab. 53. SrZrO₃. Wave numbers in 10^2 m^{-1} and symmetry of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O ₃ torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO ₃ lattice mode)
522 (B_1, B_2, A_1)	325 (B_1, B_2, A_2) (357) (379)	240 (B_1, B_2, A_1)	143 (B_1, B_2, A_1)

Nr. 1A-12 BaZrO₃, Barium zirconate

1	A few properties of BaZrO ₃ were reported in comparison with those of some perovskite-type ferroelectrics. The crystal was reported to be cubic with the cell dimensions $a = 4.192 \text{ \AA}$ at RT.	57R2
4	Linear thermal expansion: $\alpha = 5.64 \cdot 10^{-6} \text{ ^\circ C}^{-1}$ between $23 \text{ }^\circ\text{C}$ and $214 \text{ }^\circ\text{C}$; $\alpha = 6.54 \cdot 10^{-6} \text{ ^\circ C}^{-1}$ between $214 \text{ }^\circ\text{C}$ and $324 \text{ }^\circ\text{C}$ for ceramics of bulk density $\rho = 6.73 \cdot 10^3 \text{ kg m}^{-3}$.	65B10
9	Infrared absorption: Fig. 293, 294; Tab. 54.	

Tab. 54. BaZrO₃. Wave numbers in 10^2 m^{-1} and symmetries of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O ₃ torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO ₃ lattice mode)
505 (F_{1u})	- (F_{2u})	210 (F_{1u})	115 (F_{1u})

Nr. 1A-13 PbZrO₃, Lead zirconate

1a	Dielectric anomaly of PbZrO ₃ associated with a phase transition was reported independently by ROBERT and by SMOLENSKII in 1950. Antiparallel ionic shifts on the (001) projection of crystal structure were found by SAWAGUCHI et al. in 1951. In the same year antiferroelectric double hysteresis loops were discovered by SHIRANE et al.. PbZrO ₃ is the first compound in which double hysteresis loops were observed.	50R1, 50S7 51S3 51S8
b.	phase	II ^{a)}
	state	A ^{b)}
	crystal system	orthorhombic ^{c)}
	space group	Pba2-C _{2v} ^{c)}
	Θ	230 $^\circ\text{C}^a)$
		$a = 5.87 \text{ \AA}, b = 11.74 \text{ \AA}, c = 8.20 \text{ \AA}$ at RT (in phase II). The cubic unit cell in phase I becomes pseudo-tetragonal in phase II. The pseudo-tetragonal cell constants a' and c' are related with the orthorhombic cell constants a , b and c : $a = \sqrt{2} a'$, $b = 2\sqrt{2} a'$ and $c = 2c'$, where $a' = 4.15 \text{ \AA}$, $c' = 4.10 \text{ \AA}$ at RT. Relation between the pseudo-tetragonal and orthorhombic cells: Fig. 295.
		Crystal growth: PbCl ₂ flux method.

Figuren S. 271ff.

II 1 Oxide des Perowskit-Typs

3	Nr. 1A-13 PbZrO ₃ , continued Z = 8 (in phase II). The crystal is polar along the c axis and antipolar along the a axis in phase II. Fig. 295 shows schematically the shifts of Pb ions. Positional parameters and shifts from ideal perovskite positions: Tab. 55. Projection of ZrO ₆ : Fig. 296, 297, 298. Bond distances between Zr and O: Fig. 299.	51S3, 57J4, 51S3 57J4
4	Thermal expansion: Fig. 300 ... 303. $\alpha_a \cong -0.05 \cdot 10^{-5} \text{ K}^{-1}$ and $\alpha_c \cong 2.80 \cdot 10^{-5} \text{ K}^{-1}$ in phase II; $\alpha_a \cong 1.10 \cdot 10^{-5} \text{ K}^{-1}$ in phase I, where α_a and α_c are the linear thermal expansion coefficients along the pseudo-tetragonal a' and c' axes, respectively.	52S1
5a	Dielectric constants: Fig. 304. $C = 1.36 \cdot 10^5 \text{ }^{\circ}\text{K}$ (determined with ceramics). Effect of pressure: Fig. 305. $(d\Theta_a/dp)_{p \rightarrow 0} = (4.1 \pm 0.2) \cdot 10^{-8} \text{ }^{\circ}\text{K N}^{-1} \text{ m}^2$.	50R1 66R2
c	Critical field: Fig. 306.	
6a	Specific heat: Fig. 307. For the transition II-I: $\Delta Q_m = 440 \text{ cal mol}^{-1}$; $\Delta S_m = 0.88 \text{ cal }^{\circ}\text{K}^{-1} \text{ mol}^{-1}$.	
b	Thermal conductivity: Fig. 308.	52S2
8	Elastic compliances: Fig. 309.	
9a	Birefringence: Fig. 310. Infrared absorption: Fig. 311, 312; Tab. 56.	
16	Radiation damage: Fig. 313.	

Tab. 55. PbZrO₃ (ceramics). Atomic coordinates and shifts from ideal perovskite positions at RT. [57J4]

Atom	x	y	z	Wyckoff notation	Total shift Å
Pb'	0.706	0.127	0	4c	0.26
Pb''	0.706	0.127	0.500	4c	0.26
Zr'	0.243	0.124	0.250	4c	0.04
Zr''	0.243	0.124	0.250	4c	0.04
O(1)'	0.270	0.150	0.980	4c	0.35
O(1)''	0.270	0.100	0.480	4c	0.35
O(2)'	0.040	0.270	0.300	4c	0.53
O(2)''	0.040	0.270	0.750	4c	0.34
O(3)'	0	0.500	0.250	2b	0
O(3)''	0	0.500	0.800	2b	0.41
O(4)'	0	0	0.250	2a	0
O(4)''	0	0	0.800	2a	0.41

Tab. 56. PbZrO₃. Wave numbers in 10^2 m^{-1} and symmetries of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O ₃ torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO ₃ lattice mode)
508 (E_u , A ₁)	290 (B_1 , E _u)	221 (E_u , A ₁)	80 (E_u , A ₁) 34

Nr. 1A-14 PbHfO₃, Lead hafnate

1a	A dielectric anomaly associated with a phase transition was observed, and the possibility of the antiferroelectricity was discussed by SHIRANE et al. in 1953.	53S3
b	phase III (A) state II P crystal system tetragonal cubic Θ 163 215 °C	53S3
	Lattice constants for the pseudo-tetragonal phase: $a' = 4.136 \text{ \AA}$, $c'/a' = 0.991$ at RT.	53S3

4	Thermal expansion: Fig. 314. Cubic thermal expansion coefficients: below 158 °C: $20 \cdot 10^{-6}$ deg $^{-1}$; above 215 °C: $27 \cdot 10^{-6}$ deg $^{-1}$.	53S3																														
5a	Dielectric constant: Fig. 315. $C = 9.5 \cdot 10^4$ °K (ceramics).	53S3																														
Nr. 1A-15 BiFeO₃, Bismuth ferrite																																
1a	In 1960 ^{a)} it was pointed out on the basis of x-ray studies of the solid solution, PbTiO ₃ -BiFeO ₃ , that BiFeO ₃ could have a ferroelectric Curie point at high temperatures. The Curie point was estimated to be about 850 °C from studies of the same solid solution ^{b)} . Disagreement, however, exists among many experimental data reported so far, therefore reservation is necessary in deciding whether BiFeO ₃ is ferroelectric or anti-ferroelectric. Antiferromagnetic anomaly in BiFeO ₃ was observed by direct magnetic measurements at about 370 °C ^{c)} .	^{a)} 60F9, 60V2 ^{b)} 61F3, 62F8 ^{c)} 62S10, 63R1, 65I2																														
b	<table border="1"> <thead> <tr> <th>phase</th> <th>IV</th> <th>III</th> <th>II</th> <th>I</th> </tr> </thead> <tbody> <tr> <td>state</td> <td>(A) or (F), A_{magn}^*</td> <td>(A) or (F), P_{magn}</td> <td>(A) or (F), P_{magn}</td> <td>(P), P_{magn}</td> </tr> <tr> <td>crystal system</td> <td>rhombohedral</td> <td>rhombohedral</td> <td>rhombohedral</td> <td>cubic (possibly)</td> </tr> <tr> <td>space group</td> <td>R3m-C_{3v}^{***}</td> <td></td> <td></td> <td></td> </tr> <tr> <td>Θ</td> <td>370</td> <td>≈ 575</td> <td>850</td> <td>°C</td> </tr> </tbody> </table> <p>$a = (3.962 \pm 0.001)$ Å, $\alpha = 89^\circ 31' \pm 3'$ at RT. Further references are available on unit cell parameters.</p>	phase	IV	III	II	I	state	(A) or (F), A_{magn}^*	(A) or (F), P_{magn}	(A) or (F), P_{magn}	(P), P_{magn}	crystal system	rhombohedral	rhombohedral	rhombohedral	cubic (possibly)	space group	R3m-C _{3v} ^{***}				Θ	370	≈ 575	850	°C	64T6 60V2, 60F6, 60Z2					
phase	IV	III	II	I																												
state	(A) or (F), A_{magn}^*	(A) or (F), P_{magn}	(A) or (F), P_{magn}	(P), P_{magn}																												
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space group	R3m-C _{3v} ^{***}																															
Θ	370	≈ 575	850	°C																												
3	Crystal structure: From the x-ray diffraction studies, BiFeO ₃ was found to belong to one of the five space groups: R 3, R $\bar{3}$, R 32, R3m and R $\bar{3}$ m. Neutron diffraction studies suggested that BiFeO ₃ belongs to the non-centrosymmetric space group R3m. The crystal structure can be regarded as consisting of alternating FeO ₃ and BiO ₃ trigonal pyramids: Fig. 316; Tab. 57. According to the electron diffraction study, BiFeO ₃ belongs to the non-centrosymmetric space group R3m at RT. Atomic coordinates: Tab. 58. The space group R $\bar{3}$ m was, however, rejected by SMOLENSKII et al., because it does not satisfy the conditions for the existence of weak ferromagnetism. The magnetic structure of BiFeO ₃ was proved to be G-type by the neutron diffraction experiments. Fig. 317, 318.	63K5 64T6 64S9, 63K5																														
4	Unit cell parameters: Fig. 319, 320. See also	66R8, 64T5																														
5a	Dielectric constant: Fig. 321, 322, 323. No reliable data on the dielectric constant in the high temperature region near 850 °C are available.																															
11	Magnetic susceptibility: Fig. 324. At RT, no spontaneous magnetic moment was observed in the fields up to 22 kOe.																															
12c	Mössbauer effect: Fig. 325, 326.																															
17	Calculations of the internal electric fields and their gradients in BiFeO ₃ crystals were made on the basis of an ionic model.	67T7																														
<p>Tab. 57. BiFeO₃. Values of the interatomic distances [Å]. [63K5]. See Fig. 316. See also [64T6]</p> <table border="1"> <thead> <tr> <th></th> <th>520 °C</th> <th>20 °C</th> </tr> </thead> <tbody> <tr> <td>Bi-Fe (A)</td> <td>3.841</td> <td>3.857</td> </tr> <tr> <td>Bi-Fe (B)</td> <td>3.006</td> <td>2.994</td> </tr> <tr> <td>Bi-O (C)</td> <td>2.903</td> <td>2.907</td> </tr> <tr> <td>Bi-O (D)</td> <td>2.680</td> <td>2.693</td> </tr> <tr> <td>Fe-O (F)</td> <td>2.233</td> <td>2.214</td> </tr> <tr> <td>Fe-O (G)</td> <td>1.754</td> <td>1.774</td> </tr> <tr> <td>O-O (H)</td> <td>2.841</td> <td>2.859</td> </tr> <tr> <td>O-O (K)</td> <td>2.800</td> <td>2.800</td> </tr> <tr> <td>O-O (L)</td> <td>2.680</td> <td>2.724</td> </tr> </tbody> </table>				520 °C	20 °C	Bi-Fe (A)	3.841	3.857	Bi-Fe (B)	3.006	2.994	Bi-O (C)	2.903	2.907	Bi-O (D)	2.680	2.693	Fe-O (F)	2.233	2.214	Fe-O (G)	1.754	1.774	O-O (H)	2.841	2.859	O-O (K)	2.800	2.800	O-O (L)	2.680	2.724
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<p>* This state is presumably weak ferromagnetic. [66Y2] ** See subsection 3.</p>																																

Tab. 58. BiFeO₃. Atomic coordinates. [64T6]

Atom	x	y	z
Bi	0.0337	0.0337	0.0337
Fe	0.5000	0.5000	0.5000
O(1)	-0.0280	0.5000	0.5000
O(2)	0.5000	-0.0280	0.5000
O(3)	0.5000	0.5000	-0.0280

* This state is presumably weak ferromagnetic. [66Y2]

** See subsection 3.

Nr. 1A-16 KIO_3 , Potassium iodate

1a	Ferroelectric behavior in KIO_3 was reported by HERLACH in 1961.						
b	phase	V ^{a)}	IV ^{a)}	III ^{a)}	II ^{a)}	I ^{a)}	61H3 a) 61H3
	state		F ^{a)}	F ^{a)}	F ^{a)}	P ^{a)}	
	crystal system			trigonal ^{b)*}		trigonal ^{a)}	b) 60S5
	Θ	-190 ^{a)}	-18, -10 ^{a)**}	70 ^{a)}	212 ^{a)}	°C	
							66H17 08g1
							60S5 65F3
2a	Hydrothermal method: Fig. 327. Growth from the supersaturated solution with 10 ... 14% HIO_3 at a constant temperature: Fig. 328.						61H3 27m1
3	$Z = 1$ in phase III, adopting trigonal system. $Z = 8$ in phase III, adopting triclinic system.						61H3 65F3
4	Lattice deformation: $a = [4.44 + 0.00022(T - 220)] \text{ \AA}$, $\alpha = 89^\circ 20' - 0.09(T - 220)'$ in phase I (T in °C).						61H3
5a	Dielectric constants: Fig. 329, 330.						66H17
c	Spontaneous polarization: Fig. 331.						61H3
9a	Absorption edge: Fig. 332.						67V2
12a	NMR: Fig. 333.						61H3

1B Complex perovskite-type oxides

Nr. 1B1-i $(\text{K}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$, Potassium bismuth titanate

1a	Ferroelectricity in $(\text{K}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$ was found by SMOLENSKII and AGRANOVSKAYA in 1959.						59S6
b	phase	III	II	I			
	state	(F)	(A)	P			
	crystal system	tetragonal	pseudo-cubic	cubic			62I5
	space group			Pm3m-O _h ⁴			
	Θ	270	410, 380 ^{a)}	°C			a) 60S6
3	Crystal structure: Disordered perovskite.						62I5
4	Lattice distortion: Fig. 334. Thermal expansion: Fig. 335.						
5a	Dielectric constant: Fig. 336.						

Nr. 1B1-ii $(\text{Na}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$, Sodium bismuth titanate

1a	Ferroelectricity in $(\text{Na}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$ was found by SMOLENSKII and AGRANOVSKAYA in 1959.						59S6

* Various crystal systems have been proposed: trigonal [60S5], triclinic [65F3].
** -10 °C on heating, -18 °C on cooling.

II 1 Perovskite-type oxides

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1b	phase	III	II	I	
	state	F	(A)	P	
	crystal system	rhombohedral	pseudo-cubic	cubic	62I5
	space group			Pm3m-O _h ¹	
	Θ	$\approx 200^a)$	320	°C	^{a) 60S6}
	$a = (3.891 \pm 0.002) \text{ \AA}$, $\alpha = 89^\circ 36' \pm 3'$ at RT.				
3	Crystal structure: Disordered perovskite.				62I5
4	Thermal expansion: Fig. 337.				
5a	Dielectric constant: Fig. 338.				
c	Spontaneous polarization and coercive field: $P_s \approx 8.0 \cdot 10^{-2} \text{ C m}^{-2}$; $E_c \approx 14 \cdot 10^2 \text{ kV m}^{-1}$ at 116 °C.				60S6

Nr. 1B2-i $\text{Pb}(\text{Mg}_{1/2}\text{W}_{1/2})\text{O}_3$

1a	Antiferroelectric properties of $\text{Pb}(\text{Mg}_{1/2}\text{W}_{1/2})\text{O}_3$ were discovered by SMOLENSKII et al. in 1959.	59S7		
b	phase	II	I	
	state	A	P	
	crystal system	orthorhombic	cubic	62Z1
	space group	C222 ₁ -D ₂ ⁵		
	Θ	38	°C	
	$a = 22.74 \text{ \AA}$, $b = 22.79 \text{ \AA}$, $c = 15.90 \text{ \AA}$ at RT. Orthorhombic unit cell: see Fig. 339.			
2a	Crystal growth: Crystal growth of $\text{Pb}(\text{Mg}_{1/2}\text{W}_{1/2})\text{O}_3$ was reported by MYL'NIKOVA.	60M2		
3	Crystal structure: $\text{Pb}(\text{Mg}_{1/2}\text{W}_{1/2})\text{O}_3$ has the structure of perovskite type. Fig. 339. $Z = 64$ (molecular unit: Pb_2MgWO_6).	62Z1		
4	Lattice distortion associated with the phase transition. Thermal expansion: Fig. 340.	62Z1		
5a	Dielectric constants: Fig. 341, 342, 343. $d\Theta_a/dp = -5.84 \cdot 10^8 \text{ K N}^{-1}\text{m}^2$.			
6	Specific heat: Fig. 344. Transition heat (II → I): $\Delta Q_m = 276 \text{ cal mol}^{-1}$.	66S28		
8a	Elastic compliance: Fig. 345. Ultrasound absorption: Fig. 346, 347.			

Nr. 1B2-ii $\text{Pb}(\text{Cd}_{1/2}\text{W}_{1/2})\text{O}_3$

1a	Synthesis of $\text{Pb}(\text{Cd}_{1/2}\text{W}_{1/2})\text{O}_3$ was reported by BELYAEV et al. in 1963.	63B3		
b	phase	II	I	
	state	(A)	P	
	crystal system	monoclinic	cubic	
	Θ	400	°C	65F4
	$a = (4.156 \pm 0.002) \text{ \AA}$, $b = (4.074 \pm 0.002) \text{ \AA}$, $\beta = 91^\circ 9' \pm 5'$ at RT. ROGINSKAYA and VENEVTSEV reported that another transition exists at 120 °C, in addition to the transition at 400 °C.			65R4
3	Crystal structure: Superstructure lines, indicating ordered location of the octahedral voids of the perovskite lattice, were observed.	65F4		
4	Lattice distortion: Fig. 348, 349.			
5a	Dielectric constant: Fig. 350.			

Figuren S. 280 ff.

II 1 Oxide des Perowskit-Typs

Nr. 1B2-iii $\text{Pb}(\text{Mn}_{1/2}\text{W}_{1/2})\text{O}_3$

1a	A synthesis of $\text{Pb}(\text{Mn}_{1/2}\text{W}_{1/2})\text{O}_3$ was reported by VENEVSEV et al.				64V3				
b	<table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;">II</th> <th style="text-align: center;">I</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">(A), P_{magn}</td> <td style="text-align: center;">P, P_{magn}</td> </tr> </tbody> </table>				II	I	(A), P_{magn}	P, P_{magn}	65R5
II	I								
(A), P_{magn}	P, P_{magn}								
state	monoclinic	cubic							
Θ	423	$^{\circ}\text{K}$							
$a = 4.063 \text{ \AA}, b = 4.033 \text{ \AA}, \beta = 90^\circ 12'$ at RT.									
5a	Dielectric constant: Fig. 351.				65R5				
10	Electrical conductivity: $\sigma = 8 \cdot 10^{-8} \Omega^{-1} \text{ m}^{-1}$.				65R5				
11	Magnetic susceptibility: see Fig. 351.								

Nr. 1B2-iv $\text{Pb}(\text{Co}_{1/2}\text{W}_{1/2})\text{O}_3$

1a	Antiferro- and ferroelectric properties in $\text{Pb}(\text{Co}_{1/2}\text{W}_{1/2})\text{O}_3$ were discovered by FILIP'EV et al.				63F1												
b	<table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;">IV</th> <th style="text-align: center;">III</th> <th style="text-align: center;">II</th> <th style="text-align: center;">I</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">F, F_{magn} (weak)</td> <td style="text-align: center;">F, P_{magn}</td> <td style="text-align: center;">A, P_{magn}</td> <td style="text-align: center;">P, P_{magn}</td> </tr> </tbody> </table>				IV	III	II	I	F, F_{magn} (weak)	F, P_{magn}	A, P_{magn}	P, P_{magn}	65B8				
IV	III	II	I														
F, F_{magn} (weak)	F, P_{magn}	A, P_{magn}	P, P_{magn}														
state			orthorhombic	cubic													
Θ	9 ^{a)}	83 ... 103	293 ^{b)}	$^{\circ}\text{K}$													
			305														
$a = 4.008 \text{ \AA}$ at $298 \text{ }^{\circ}\text{K}$.																	
2a	Crystal growth: Flux method with PbO .				65B8												
3	Crystal structure: A superstructure was observed which was completely explained by alternation of the population of the oxygen octahedra by Co^{2+} and W^{6+} cations along the three directions. The real elementary lattice is a cubic face centered one with the parameter $A = 2a$ for phase I and with the parameters $A = 2 \cos(\beta/2)$, $B = 2b$, and $C = 2a \sin(\beta/2)$ for II, where a , b and β are the parameters of the perovskite sub-lattice.				64F4												
4	<table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;">phase</th> <th colspan="3" style="text-align: center;">lattice parameters</th> </tr> </thead> <tbody> <tr> <td>I</td> <td colspan="3">$A = 8.017 \text{ \AA}$ at $298 \text{ }^{\circ}\text{K}$</td> </tr> <tr> <td>II</td> <td colspan="3">$A = 5.669 \text{ \AA}, B = 7.956 \text{ \AA}, C = 5.689 \text{ \AA}$ at $258 \text{ }^{\circ}\text{K}$</td> </tr> </tbody> </table> <p>Lattice distortion: Fig. 352.</p>				phase	lattice parameters			I	$A = 8.017 \text{ \AA}$ at $298 \text{ }^{\circ}\text{K}$			II	$A = 5.669 \text{ \AA}, B = 7.956 \text{ \AA}, C = 5.689 \text{ \AA}$ at $258 \text{ }^{\circ}\text{K}$			64F4
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5a	Dielectric constant: Fig. 353, 354, 355.																
c	Polarization: Fig. 356.																
11	Magnetic susceptibility and magnetization: Fig. 357, 358.																

Nr. 1B2-v $\text{Pb}(\text{Mn}_{1/2}\text{Re}_{1/2})\text{O}_3$

1a	A synthesis of $\text{Pb}(\text{Mn}_{1/2}\text{Re}_{1/2})\text{O}_3$ was reported by VENEVSEV et al.				64V3						
b	<table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;">III</th> <th style="text-align: center;">II</th> <th style="text-align: center;">I</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">(A), F_{magn}</td> <td style="text-align: center;">(A), P_{magn}</td> <td style="text-align: center;">P, P_{magn}</td> </tr> </tbody> </table>				III	II	I	(A), F_{magn}	(A), P_{magn}	P, P_{magn}	65R5
III	II	I									
(A), F_{magn}	(A), P_{magn}	P, P_{magn}									
state	monoclinic	cubic									
Θ	103	393	$^{\circ}\text{K}$								
$a = 4.043 \text{ \AA}, b = 4.012 \text{ \AA}, \beta = 90^\circ 33'$ at RT.											
3	Crystal structure: Ordered perovskite.				65R5						

4	Lattice distortion: Fig. 359.	65R5																				
10	Electrical conductivity: $\sigma = 1 \cdot 10^{-1} \Omega^{-1} m^{-1}$.	65R5																				
11	Magnetic susceptibility and magnetic moment: Fig. 360. The linear temperature dependence of χ_{magn}^{-1} with a positive value of $\Theta_{\text{pmagn}} = 85 \text{ }^{\circ}\text{K}$, and the appearing of the spontaneous moment at $103 \text{ }^{\circ}\text{K}$, may indicate the presence of ferromagnetic properties in this compound, which is in agreement with the positive sign of the indirect exchange interaction proposed by GOODENOUGH for Mn^{2+} and Re^{6+} ions. However, the magnitudes of the calculated theoretical spontaneous moments agree with the experimental values only on the assumption of an anti-ferromagnetic interaction between ions distributed in an ordered fashion over the octahedral vacancies.	65R5																				
Nr. 1B3-i $\text{Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$																						
1a	Ferroelectricity in $\text{Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$ was discovered by SMOLENSKII et al. in 1959.	59S9																				
b	<table border="1"> <tr> <td>phase</td> <td>II</td> <td>I</td> </tr> <tr> <td>state</td> <td>F</td> <td>P</td> </tr> <tr> <td>crystal system</td> <td>tetragonal^{a)} (possibly)</td> <td>cubic</td> </tr> <tr> <td>Θ</td> <td>90</td> <td>$^{\circ}\text{C}$</td> </tr> </table>	phase	II	I	state	F	P	crystal system	tetragonal ^{a)} (possibly)	cubic	Θ	90	$^{\circ}\text{C}$	59S9								
phase	II	I																				
state	F	P																				
crystal system	tetragonal ^{a)} (possibly)	cubic																				
Θ	90	$^{\circ}\text{C}$																				
	$a = (4.074 \pm 0.001) \text{ \AA}$, $c = (4.083 \pm 0.001) \text{ \AA}$ at RT. ^{a)}	^{a)} 60I3																				
3	Crystal structure: In the powder patterns, additional to the principal lines of the perovskite structure, superstructural lines were observed indicating a doubling of the lattice period.	59I3																				
5a	Dielectric constant: Fig. 361.																					
c	Spontaneous polarization: $P_s \approx 3.6 \cdot 10^{-2} \text{ cm}^{-2}$ at $18 \text{ }^{\circ}\text{C}$.	59S9																				
Nr. 1B3-ii $\text{Pb}(\text{Mn}_{1/2}\text{Nb}_{1/2})\text{O}_3$																						
1a	A synthesis of $\text{Pb}(\text{Mn}_{1/2}\text{Nb}_{1/2})\text{O}_3$ with perovskite structure was reported by VENEV-TSEV et al.	64V3																				
Nr. 1B3-iii $\text{Pb}(\text{Fe}_{1/2}\text{Nb}_{1/2})\text{O}_3$																						
1a	Ferroelectricity in $\text{Pb}(\text{Fe}_{1/2}\text{Nb}_{1/2})\text{O}_3$ was discovered by SMOLENSKII et al. in 1958.	58S4																				
b	<table border="1"> <tr> <td>phase</td> <td>III</td> <td>II</td> <td>I</td> </tr> <tr> <td>state</td> <td>F, A_{magn}</td> <td>F, P_{magn}</td> <td>P, P_{magn}</td> </tr> <tr> <td>crystal system</td> <td>rhombohedral</td> <td>rhombohedral</td> <td>cubic</td> </tr> <tr> <td>space group</td> <td></td> <td></td> <td>Pm3m-O_h^1</td> </tr> <tr> <td>Θ</td> <td>143</td> <td>387</td> <td>$^{\circ}\text{K}$</td> </tr> </table>	phase	III	II	I	state	F, A_{magn}	F, P_{magn}	P, P_{magn}	crystal system	rhombohedral	rhombohedral	cubic	space group			Pm3m- O_h^1	Θ	143	387	$^{\circ}\text{K}$	62B7 64S8 62B10
phase	III	II	I																			
state	F, A_{magn}	F, P_{magn}	P, P_{magn}																			
crystal system	rhombohedral	rhombohedral	cubic																			
space group			Pm3m- O_h^1																			
Θ	143	387	$^{\circ}\text{K}$																			
a	$a = 4.014 \text{ \AA}$, $\alpha = 89.92^\circ$ at RT.																					
2a	Crystal growth: Flux method with PbO .	62B7																				
3	Crystal structure: Disordered perovskite; X-ray studies have not shown any ionic ordering in the octahedral sites of perovskite structure. The magnetic peak was found in the neutron diffraction experiments at $78 \text{ }^{\circ}\text{K}$. The effective magnetic moment of the Fe^{3+} ion was found to be $(0.80 \pm 0.16) \mu_B$ at $78 \text{ }^{\circ}\text{K}$ from the calculation of the intensity of the (111) reflection, which is about 90% of the magnetic moment at $0 \text{ }^{\circ}\text{K}$. Fig. 362.	64S8 65D6																				
5a	Dielectric constant: Fig. 363.																					
9a	Optical absorption: Fig. 364.																					
11	Magnetic susceptibility: Fig. 365. $\mu_{\text{eff}} = 5.4 \mu_B$.	62B7																				
12b	ESR: Fig. 366.																					
c	Mössbauer effect: Fig. 367, 368. The quadrupole splitting $\Delta E_{\text{qu}} = (0.37 \pm 0.02) \text{ mm sec}^{-1}$, the isomer shift $\delta = (0.52 \pm 0.02) \text{ mm sec}^{-1}$, corresponding to trivalent iron (at $20 \text{ }^{\circ}\text{C}$).	66S22																				

Figuren S. 283

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			1b												
			4												
			5a												
			Nr.												
			1a												
			b												
			3												
			5a												
			Nr.												
			1a												
			b												
			Nr.												
			1a												
			b												
			2a												
			3												
			4												
			5a												
			c												
			11												
Nr. 1B3-iv $Pb(Co_{1/2}Nb_{1/2})O_3$															
1a	A synthesis of $Pb(Co_{1/2}Nb_{1/2})O_3$ with perovskite structure was reported by VENEV-TSEV et al.	64V3													
b	Informations on the dielectric and magnetic properties are available:	65R5													
Nr. 1B3-v $Pb(Ni_{1/2}Nb_{1/2})O_3$															
1a	$Pb(Ni_{1/2}Nb_{1/2})O_3$ with perovskite structure was synthesized by the addition of 5 mol % BaO.	65S17													
Nr. 1B3-vi $Pb(In_{1/2}Nb_{1/2})O_3$															
1a	Dielectric anomaly in $Pb(In_{1/2}Nb_{1/2})O_3$ was found by KUPRIYANOV and FESENKO in 1965.	65K9													
b	<table border="1"> <tr> <td>phase</td> <td>II</td> <td>I</td> </tr> <tr> <td>state</td> <td>(F)</td> <td>P</td> </tr> <tr> <td>crystal system</td> <td>monoclinic (possibly)</td> <td>cubic</td> </tr> <tr> <td>Θ</td> <td>90</td> <td>°C</td> </tr> </table> $a = 4.11 \text{ \AA}$ at RT.	phase	II	I	state	(F)	P	crystal system	monoclinic (possibly)	cubic	Θ	90	°C	65K9	
phase	II	I													
state	(F)	P													
crystal system	monoclinic (possibly)	cubic													
Θ	90	°C													
5a	Dielectric constant: Fig. 369.														
Nr. 1B3-vii $Pb(Yb_{1/2}Nb_{1/2})O_3$															
1a	Antiferroelectric properties in $Pb(Yb_{1/2}Nb_{1/2})O_3$ were reported by FILIP'EV et al. in 1963.	63F1													
b	<table border="1"> <tr> <td>phase</td> <td>II</td> <td>I</td> </tr> <tr> <td>state</td> <td>AF</td> <td>P</td> </tr> <tr> <td>crystal system</td> <td>monoclinic</td> <td>cubic</td> </tr> <tr> <td>Θ</td> <td>300, 310^{a)}</td> <td>°C</td> </tr> </table> $a = 4.168 \text{ \AA}$, $b = 4.107 \text{ \AA}$, $\beta = 90^\circ 27'$ at RT ^{a)} .	phase	II	I	state	AF	P	crystal system	monoclinic	cubic	Θ	300, 310 ^{a)}	°C	64T4	
phase	II	I													
state	AF	P													
crystal system	monoclinic	cubic													
Θ	300, 310 ^{a)}	°C													
3	Crystal structure: Superstructure lines, corresponding to ordering of Yb ³⁺ and Nb ⁵⁺ ions were found.	64T4													
4	Lattice distortion: Fig. 370. Thermal expansion: Fig. 371.														
5a	Dielectric constant: Fig. 372.														
Nr. 1B3-viii $Pb(Ho_{1/2}Nb_{1/2})O_3$															
1a	Dielectric anomaly in $Pb(Ho_{1/2}Nb_{1/2})O_3$ was found by KUPRIYANOV and FESENCO.	65K9													
b	<table border="1"> <tr> <td>phase</td> <td>II</td> <td>I</td> </tr> <tr> <td>state</td> <td>(A)</td> <td>P</td> </tr> <tr> <td>crystal system</td> <td>monoclinic</td> <td>cubic</td> </tr> <tr> <td>Θ</td> <td>240</td> <td>°C</td> </tr> </table> $a = 4.160 \text{ \AA}$, $b = 4.106 \text{ \AA}$, $\beta = 90^\circ 30'$ at RT.	phase	II	I	state	(A)	P	crystal system	monoclinic	cubic	Θ	240	°C	65K9	
phase	II	I													
state	(A)	P													
crystal system	monoclinic	cubic													
Θ	240	°C													
5a	Dielectric constant: Fig. 373.														
Nr. 1B3-ix $Pb(Lu_{1/2}Nb_{1/2})O_3$															
1a	Dielectric anomaly in $Pb(Lu_{1/2}Nb_{1/2})O_3$ was found by SMOLENSKII and AGRANOV-SKAYA in 1958.	58S3													

1b	phase	II	I	
	state	(A)	P	
	crystal system	monoclinic	cubic	
	Θ	270	°C	
		$a = 4.152 \text{ \AA}$, $b = 4.093 \text{ \AA}$, $\beta = 90^\circ 30'$ at RT.		65K9
4	Thermal expansion: Fig. 374.			
5a	Dielectric constant: Fig. 375.			

Nr. 1B3-x $\text{Pb}(\text{Sc}_{1/2}\text{Ta}_{1/2})\text{O}_3$

1a b	Ferroelectricity in $\text{Pb}(\text{Sc}_{1/2}\text{Ta}_{1/2})\text{O}_3$ was discussed by SMOLENSKII et al. in 1959.	59S9		
	phase	II	I	
	state	F	P	59S9
	crystal system	tetragonal ^{a)} (possibly)	cubic	^{a)} 59I3
	Θ	26	°C	
		$a = (4.072 \pm 0.001) \text{ \AA}$, $c = (4.072 \pm 0.001) \text{ \AA}$ at RT ^{a)} .		
3	Crystal structure: The large number of superstructure lines and their great intensity in $\text{Pb}(\text{Sc}_{1/2}\text{Ta}_{1/2})\text{O}_3$ indicates that the degree of ordering of Sc^{3+} and Ta^{5+} ions is greater than in $\text{Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$. See 1B3-i-3.	59I3		
5a	Dielectric constant: Fig. 376.			

Nr. 1B3-xi $\text{Pb}(\text{Mn}_{1/2}\text{Ta}_{1/2})\text{O}_3$

1a	$\text{Pb}(\text{Mn}_{1/2}\text{Ta}_{1/2})\text{O}_3$ with perovskite structure was synthesized by the addition of 5 mol% SrO .	65S17
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Nr. 1B3-xii $\text{Pb}(\text{Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$

1a b	Ferroelectricity in $\text{Pb}(\text{Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$ was discovered by SMOLENSKII et al. in 1959.	59S7		
	phase	III	II	I
	state	F, A _{magn}	F, P _{magn}	P, P _{magn}
	crystal system	rhombohedral	rhombohedral ^{a)}	cubic
	space group			Pm3m-O _h ¹
	Θ	143, 133 ^{a)}	243, 233 ^{a)}	°K
		$P_s \parallel [111]$ (probably).		
		$a = (4.007 \pm 0.001) \text{ \AA}$ at RT.		
		black (dark orange for thin samples).		
2a	Crystal growth: Flux method with PbO . When the soak temperature is higher than 1200 °C, crystals are obtained having both pyrochloride and perovskite structure.	68N1		
3	Crystal structure: Disordered perovskite.	65S17		
4	phase	lattice constants		
I		$a = (4.007 \pm 0.001) \text{ \AA}$ at RT.		
II		$a = (4.006 \pm 0.001) \text{ \AA}$ at 90 °K $\alpha = 89.89^\circ \pm 0.02^\circ$		
5a c	Dielectric constant: Fig. 377, 378. Spontaneous polarization: Fig. 379.			
11	Magnetic susceptibility: Fig. 380. $\mu_{\text{eff}} = 5.92 \mu_B$; $\Theta_{\text{p magn}} = -370$ °K.			68N1

Figuren S. 285

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Nr. 1B3-xiii $Pb(Co_{1/2}Ta_{1/2})O_3$

1a A synthesis of $Pb(Co_{1/2}Ta_{1/2})O_3$ with perovskite structure was reported by SHVORNEVA and VENEVTSEV. The compound was stabilized by the addition of 1 mol% La_2O_3 . | 65S17

Nr. 1B3-xiv $Pb(Yb_{1/2}Ta_{1/2})O_3$

1a	Dielectric anomaly in $Pb(Yb_{1/2}Ta_{1/2})O_3$ was reported by ISUPOV and KRANIK in 1964.			64I6
b	phase	II	I	
	state	(A)	F	
	crystal system	monoclinic	cubic	
	Θ	280, 285 ^{a)} °C		
		$a = 4.154 \text{ \AA}$, $b = 4.108 \text{ \AA}$, $\beta = 90^\circ 30'$ at RT.		

4 Thermal expansion: Fig. 381.

5a Dielectric constant: Fig. 382.

Nr. 1B3-xv $Pb(Lu_{1/2}Ta_{1/2})O_3$

1a	Dielectric anomaly in $Pb(Lu_{1/2}Ta_{1/2})O_3$ was found by SMOLENSKII and AGRANOV-SKAYA in 1958.			58S3
b	phase	II	I	
	state	(A)	P	
	crystal system	monoclinic	cubic	
	Θ	280 °C		
		$a = 4.153 \text{ \AA}$, $b = 4.107 \text{ \AA}$, $\beta = 90^\circ 30'$ at RT.		
4	Lattice distortion: Fig. 383. Thermal expansion: Fig. 384.			
5	Dielectric constant: Fig. 385.			

Nr. 1B3-xvi $Pb(Fe_{1/2}W_{1/2})O_3$

1a	A synthesis of $Pb(Fe_{1/2}W_{1/2})O_3$ with perovskite structure was reported by VENEVTSIEV et al.			64V3
b	The magnetic measurements confirmed the presence of the spinel phase in a sample of this composition.			65R5

Nr. 1B3-xvii $Pb(Li_{1/4}Nb_{1/4}W_{1/2})O_3$ and sister crystals

1a	Following composite perovskite compounds containing Pb were synthesized: $Pb(Li_{1/4}Nb_{1/4}W_{1/2})O_3$ $Pb(Zn_{1/4}Mn_{1/4}Nb_{1/2})O_3$ $Pb(Co_{1/4}Mn_{1/4}W_{1/2})O_3$ $Pb(Mg_{1/4}Mn_{1/4}Nb_{1/2})O_3$ $Pb(Cd_{1/4}Mn_{1/4}Nb_{1/2})O_3$ $Pb(Ni_{1/4}Mn_{1/4}W_{1/2})O_3$ $Pb(Co_{1/4}Mn_{1/4}Nb_{1/2})O_3$ $Pb(Mg_{1/4}Mn_{1/4}Ta_{1/2})O_3$ $Pb(Cd_{1/4}Mn_{1/4}W_{1/2})O_3$ $Pb(Ni_{1/4}Mn_{1/4}Nb_{1/2})O_3$ $Pb(Mg_{1/4}Mn_{1/4}W_{1/2})O_3$ $Pb(Sc_{1/4}Cr_{1/4}Nb_{1/2})O_3$	64V3 65V3
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Nr. 1B4-i $Pb(Mg_{1/3}Nb_{2/3})O_3$

1a	Ferroelectricity in $Pb(Mg_{1/3}Nb_{2/3})O_3$ was discovered by SMOLENSKII and AGRANOV-SKAYA in 1958.			58S3, 59S6
b	phase	II	I	
	state	F	P	
	crystal system		cubic	
	space group		Pm3m-O _h	
	Θ	265 ^{a)} °K		
		$\rho = 8.12 \cdot 10^3 \text{ kg m}^{-3}$, $a = 4.04 \text{ \AA}$ at RT. Transparent, pale yellow.		
				61B5, 60S7 a) 67B9 67B18

2a	Crystal growth: Flux method (using PbO). Kyropoulos method.	59M5 67B18
3	Crystal structure: Disordered perovskite.	61B5
4	Thermal expansion: Fig. 386.	
5a	Dielectric constant: Fig. 387, 388, 389.	
b	Nonlinear dielectric properties: $E = [(T - \Theta_p) (\epsilon_0 C)^{-1}] P + \xi P^3 + \zeta P^5 + \dots$, where $\Theta_p = 265^\circ\text{K}$, $C = (3.7 \pm 1.0) \cdot 10^5^\circ\text{K}$, and $\xi \cong 5.6 \cdot 10^8 \text{ V m}^5 \text{ C}^{-3}$.	67B9
c	Spontaneous polarization and coercive field: Fig. 390.	
7a	Piezoelectricity: Fig. 391.	
9a	Refractive index: $n = 2.56$ for 6328 \AA at 299°K . Birefringence: It was found that the crystals $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ behave like optically isotropic crystals. An applied electric field causes double refraction. Fig. 392.	67B9
e	Quadratic electrooptic effect: $M_{11} - M_{12} = +0.015 \text{ m}^4 \text{ C}^{-2}$, $M_{44} = +0.008 \text{ m}^4 \text{ C}^{-2}$ for 6328 \AA at 299°K .	67B9
14a	Domain structure: Clear domains were observed only in very thin wafers (e. g., $20 \cdot 10^{-6} \text{ m}$).	61B5

Nr. 1B4-ii $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$

1a	Ferroelectric $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$ crystal was synthesized by BOKOV and MYL'NIKOVA in 1960.	60B7												
b	<table border="1"> <tr> <td>phase</td> <td>II</td> <td>I</td> </tr> <tr> <td>state</td> <td>F</td> <td>P</td> </tr> <tr> <td>crystal system</td> <td></td> <td>cubic</td> </tr> <tr> <td>Θ</td> <td>140</td> <td>$^\circ\text{C}$</td> </tr> </table> <p>$a = 4.04 \text{ \AA}$ at RT. light yellow.</p>	phase	II	I	state	F	P	crystal system		cubic	Θ	140	$^\circ\text{C}$	60B7
phase	II	I												
state	F	P												
crystal system		cubic												
Θ	140	$^\circ\text{C}$												
2a	Crystal growth: Flux method with PbO. The crystals were separated from the matrix solution by washing in acetic acid at RT for a long time.	60B7												
5a	Dielectric constant: Fig. 393.													

Nr. 1B4-iii $\text{Pb}(\text{Cd}_{1/3}\text{Nb}_{2/3})\text{O}_3$

1b	Dielectric anomaly in $\text{Pb}(\text{Cd}_{1/3}\text{Nb}_{2/3})\text{O}_3$ was reported by VENEVTSYEV et al. in 1966.	65T5, 66V5
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Nr. 1B4-iv $\text{Pb}(\text{Co}_{1/3}\text{Nb}_{2/3})\text{O}_3$

1a	Ferroelectricity in $\text{Pb}(\text{Co}_{1/3}\text{Nb}_{2/3})\text{O}_3$ was found by BOKOV and MYL'NIKOVA in 1960.	60B7															
b	<table border="1"> <tr> <td>phase</td> <td>II</td> <td>I</td> </tr> <tr> <td>state</td> <td>F</td> <td>P</td> </tr> <tr> <td>crystal system</td> <td></td> <td>cubic</td> </tr> <tr> <td>space group</td> <td></td> <td>Pm3m-O_h</td> </tr> <tr> <td>Θ</td> <td>-98</td> <td>$^\circ\text{C}$</td> </tr> </table> <p>$a = 4.04 \text{ \AA}$ at RT. brown.</p>	phase	II	I	state	F	P	crystal system		cubic	space group		Pm3m-O _h	Θ	-98	$^\circ\text{C}$	60B7
phase	II	I															
state	F	P															
crystal system		cubic															
space group		Pm3m-O _h															
Θ	-98	$^\circ\text{C}$															
2a	Crystal growth: Flux method with PbO.	60B7															
5a	Dielectric constant: Fig. 394.																

Figuren S. 287

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Nr. 1B4-v $\text{Pb}(\text{Ni}_{1/3}\text{Nb}_{2/3})\text{O}_3$

1a	Ferroelectricity in $\text{Pb}(\text{Ni}_{1/3}\text{Nb}_{2/3})\text{O}_3$ was discovered by SMOLENSKII and AGRANOV-SKAYA in 1958.			58S3, 59S6 61B5, 60S7 59M5 59M5 59M5 61B5
b	phase	II	I	
	state	F	P	
	crystal system		cubic	
	space group		Pm3m-O _h ¹	
	Θ	153	°K	
	$a = 4.03 \text{ \AA}$ at RT. $\rho = 8.55 \cdot 10^3 \text{ kg m}^{-3}$. yellowish green.			
2a	Crystal growth: Flux method with PbO.			59M5
3	Crystal structure: Disordered perovskite.			59M5
4	Thermal expansion: Fig. 395.			59M5
5a	Dielectric constant: Fig. 396, 397, 398.			61B5
9a	Birefringence: Fig. 399.			

Nr. 1B4-vi $\text{Pb}(\text{Mg}_{1/3}\text{Ta}_{2/3})\text{O}_3$

1a	Ferroelectricity in $\text{Pb}(\text{Mg}_{1/3}\text{Ta}_{2/3})\text{O}_3$ was found by BOKOV and MYL'NIKOVA in 1960.			60B7 60B7 60B7 60B7 60B7
b	phase	II	I	
	state	F	P	
	crystal system		cubic	
	space group		Pm3m-O _h ¹	
	Θ	-98	°C	
	$a = 4.02 \text{ \AA}$ at RT. light yellow.			
2a	Crystal growth: Flux method with PbO.			60B7
3	Crystal structure: Disordered perovskite.			60B7
5a	Dielectric constant: Fig. 400.			

Nr. 1B4-vii $\text{Pb}(\text{Co}_{1/3}\text{Ta}_{2/3})\text{O}_3$

1a	Ferroelectricity in $\text{Pb}(\text{Co}_{1/3}\text{Ta}_{2/3})\text{O}_3$ was found by BOKOV and MYL'NIKOVA in 1960.			60B7 60B7 60B7 60B7 60B7
b	phase	II	I	
	state	F	P	
	crystal system		cubic	
	space group		Pm3m-O _h ¹	
	Θ	-140	°C	
	$a = 4.01 \text{ \AA}$ at RT. brown.			
2a	Crystal growth: Flux method with PbO.			60B7
3	Crystal structure: Disordered perovskite.			60B7
5a	Dielectric constant: Fig. 401.			

Nr.
1a
b
2a
3
5a
Nr.
1a
b
5a
10
11
Nr.
1a
b
2a
5a
11
12b
1C
Nr.
1b
5a
6a
7a

Nr. 1B4-viii $Pb(Ni_{1/3}Ta_{2/3})O_3$

1a	Ferroelectricity in $Pb(Ni_{1/3}Ta_{2/3})O_3$ was found by BOKOV and MYL'NIKOVA in 1960.			60B7
b	phase	II	I	
	state	F	P	
	crystal system		cubic	
	space group		Pm3m-O _b ¹	
	Θ	-180	°C	

$a = 4.01 \text{ \AA}$ at RT.
green.

2a Crystal growth: Flux method.

3 Crystal structure: Disordered perovskite.

5a Dielectric constant: Fig. 402.

Nr. 1B5-i $Pb(Mn_{2/3}W_{1/3})O_3$

1a	Dielectric and magnetic anomalies in $Pb(Mn_{2/3}W_{1/3})O_3$ were reported by ROGINSKAYA et al. in 1965.			65R5
b	phase	III	II	I
	state	(A), (A _{magn})	(A), P _{magn}	P, P _{magn}
	crystal system		monoclinic	cubic
	Θ	203	473	°K
	$a = c = 4.098 \text{ \AA}, b = 4.014 \text{ \AA}, \beta = 90^\circ 23'$ at RT.			

5a Dielectric constant: Fig. 403.

10 $\sigma = 2 \cdot 10^{11} \Omega^{-1} \text{ m}^{-1}$.11 Magnetic susceptibility: see Fig. 403.
 $\Theta_{p\ magn} = -75 \text{ }^\circ\text{K}$.**Nr. 1B5-ii $Pb(Fe_{2/3}W_{1/3})O_3$**

1a	Ferroelectricity in $Pb(Fe_{2/3}W_{1/3})O_3$ was discovered by SMOLENSKII et al. in 1959.			59S7
b	phase	III	II	I
	state	F, A _{magn}	P, A _{magn}	P, P _{magn}
	crystal system		cubic	cubic
	Θ	178	363	°K
	$a = 4.02 \text{ \AA}$ at RT.			

2a Flux method (PbO).

5a Dielectric constant: Fig. 404.

11 Magnetic susceptibility: see Fig. 404.
Magnetization is a linear function of the magnetic field intensity up to 8000 Oe.
Effective magnetic moment: $4.2 \mu_B$.

12b ESR: Fig. 405.

1C Solid solutions with perovskite-type oxides as end members**Nr. 1C-a1 $NaNbO_3$ - $KNbO_3$**

1b	Phase diagram: Fig. 406, 407, 408. Lattice parameters: Fig. 409.	
5a	Dielectric constant: Fig. 410; see Tab. 60. Polarization and coercive field: Fig. 411.	
6a	Transition energy: Tab. 59.	
7a	Electromechanical properties: Fig. 412 ... 417; Tab. 60.	

Tab. 59. $(Na_{1-x}K_x)NbO_3$. Transition energy AQ_m . [54S3]

x	Lower phase change	Upper phase change
1.00 ($KNbO_3$)	85 cal/mole	190 cal/mole
0.10	20 cal/mole	60 cal/mole
0 ($NaNbO_3$)	—	50 cal/mole

Tab. 60. $(Na_{0.5}K_{0.5})NbO_3$ (ceramics). Electric and electromechanical constants. [59E1]

Dielectric constant (100 kHz)	290
Dissipation factor (100 kHz)	$\approx 4.0\%$
Specific resistivity ρ	$10^{10} \Omega m$
Density ρ	$4.25 \cdot 10^3 \text{ kg m}^{-3}$
Poisson's ratio (assumed)	0.27
Coupling factor k_p	$0.34 \dots 0.39$
Frequency constant f_R	1.67 kHz m
Mechanical Q_{mech} (radial)	130
Young's modulus E	$1.04 \cdot 10^{11} \text{ N m}^{-2}$
Piezoelectric constant $-d_{31}$	$32 \cdot 10^{-12} \text{ C N}^{-1}$
Piezoelectric constant $-g_{31}$	$12.6 \cdot 10^{-3} \text{ m}^2 \text{ C}^{-1}$
Piezoelectric constant d_{33}^*	$80 \cdot 10^{-12} \text{ C N}^{-1}$
Piezoelectric constant g_{33}^*	$31.5 \cdot 10^{-3} \text{ m}^2 \text{ C}^{-1}$
Coupling factor k_{33}^*	0.51

Nr. 1C-a2 $NaNbO_3$ - $NaTaO_3$

1b | Phase diagram: Fig. 418.

Lattice parameters: Fig. 419.

4 | Thermal expansion: Fig. 420.

5a | Dielectric constant: Fig. 421.

9a | Birefringence: Fig. 422.

Nr. 1C-a3 $NaNbO_3$ - $NaSbO_3$

1a | Curie temperature: Fig. 423.

Nr. 1C-a4 $KNbO_3$ - $KTaO_3$

1 | Phase diagram: Fig. 424, 425.

5a | Dielectric properties: Fig. 426, 427.
 Θ_f : see Tab. 61.

6 | Thermal properties: Fig. 428; Tab. 61.

9 | See 1C-a5 for optical properties of $K(Ta_{0.35}Nb_{0.65})O_3$ (KTN).Tab. 61. $K(Nb_{1-x}Ta_x)O_3$. L : latent heat, Θ_f : Curie point, A : constant in the formula for free energy = $A(T - \Theta_p)P^2 + \dots$, P_{calc} : P_s calculated for $T = \Theta_f$. [59H1]

x	L cal mol $^{-1}$	Θ_f °K	A 10 5 °K $^{-1}$	P_{calc} 10 2 C m $^{-2}$
0	110 \pm 10	679	2.6	27
0.06	46 \pm 4	656	2.7	17.7
0.12	10 \pm 2	623	2.85	7.9
0.18	4.0 \pm 2	591	3.05	5.1

Nr. 1C-a5 $K(Ta_{0.35}Nb_{0.65})O_3$ (KTN)For general properties of $KNbO_3$ - $KTaO_3$ see 1C-a4.

9b | Electroreflectance: Fig. 429.

d | Faraday rotation: Fig. 430. See also Tab. 44.

Nr. 1C-a6 $CaTiO_3$ - $SrTiO_3$ 1b | Phase diagram: Fig. 431, 432, 433.
Lattice parameters: Fig. 434.

5a | Dielectric constant: Fig. 435, 436.

c | Spontaneous polarization: Fig. 437.

Nr. 1C-a7 $CaTiO_3$ - $BaTiO_3$ 1b | Phase diagram: Fig. 438, 439, 440.
Lattice parameters: Fig. 441.

5a | Dielectric constant: Fig. 442, 443.

6b | Thermal conductivity: Fig. 444.

7a | Electromechanical property: Tab. 62. See Fig. 183 and Tab. 40.

* Estimated values.

Nr.
Nr.

Tab

Poly

Sing

Nr.

Nr.

V

Tab. 62. $(\text{Ba}_{1-x}\text{Ca}_x)\text{TiO}_3$ (ceramics, pure BaTiO_3 base). d_{31} and d_{33} at RT. [57B4]

x	ρ 10^3 kg m^{-3}	ρ_x 10^3 kg m^{-3}	d_{31} $10^{-12} \text{ C N}^{-1}$	d_{33} $10^{-12} \text{ C N}^{-1}$	$-d_{33}/d_{31}$	Porosity $(1 - (\rho/\rho_x))$
0	5.85	6.017	-97.5	229	2.35	0.028
0.05	5.70	5.85	-66.6	167	2.51	0.026
0.07	5.68	5.80	-58.0	150	2.58	0.021
0.09	5.65	5.74	-52.1	139	2.67	0.016
0.12	5.55	5.66	-43.4	124.5	2.88	0.019

Nr. 1C-a8 $\text{CaTiO}_3\text{-PbTiO}_3$ 1b | Curie temperature: Fig. 445.
Lattice parameter: Fig. 446.**Nr. 1C-a9** $\text{SrTiO}_3\text{-BaTiO}_3$ 1b | Phase diagram: Fig. 447 ... 450.
Lattice parameter: Fig. 451; see Fig. 448.5a | Dielectric constant: Fig. 452.
Microwave dielectric loss: Tab. 63.

6a | Specific heat: Fig. 453.

10b | Conductivity associated with doping: Fig. 454, 455, 456.

Tab. 63. $(\text{Ba}_{1-x}\text{Sr}_x)\text{TiO}_3$. Dielectric loss: α, β, γ at 20 GHz. [62R4]. $(T - \Theta_p) \tan \delta = \alpha + \beta T + \gamma T^2$.

Sample		Heat treatment	Grain size μ	Θ_p $^\circ\text{K}$	α $^\circ\text{K}$	$\beta \cdot 10^4$ $(^\circ\text{K})^{-1}$	$\gamma \cdot 10^6$ $(^\circ\text{K})^{-1}$
Polycrystalline	SrTiO_3	Hot pressed and fired in air at 900 °C for 10 h	1	37	0.33	7.7	4.3
		Refired at 1200 °C in air for 10 h	3	37	0.26	5.5	4.7
		Refired at 1400 °C in air for 10 h	15	37	0.17	4.4	4.2
		Refired at 1500 °C in O_2 for 6 h	30	37	0.08	4.5	3.7
	$\text{Ba}_{0.2}\text{Sr}_{0.8}\text{TiO}_3$	Hot pressed and fired in O_2 at 1500 °C for 10 h	30	105	0.6	9	2.5
	$\text{Ba}_{0.5}\text{Sr}_{0.5}\text{TiO}_3$	Hot pressed and fired in O_2 at 1500 °C for 10 h	30	218	2.0	(9) ^{a)}	(2.5)
	$\text{Ba}_{0.7}\text{Sr}_{0.3}\text{TiO}_3$	Ceramic fired to 1375 °C in air for 1 h	8	280	2.2	(9)	(2.5)
	$\text{Ba}_{0.8}\text{Sr}_{0.2}\text{TiO}_3$	Ceramic fired to 1300 °C in air for 1 h	8	324	1.6	(9)	(2.5)
Single crystal	SrTiO_3	None	∞	37	0	6.53	2.54
	$\text{SrTiO}_3 + 0.1\% \text{Gd}^{3+}$	None	∞	37	0.033	(6.53)	(2.54)
	$\text{SrTiO}_3 + 0.03\% \text{Fe}^{3+}$	None	∞	37	0.043	(6.53)	(2.54)

Nr. 1C-a10 $\text{SrTiO}_3\text{-PbTiO}_3$ 1b | Curie temperature: Fig. 457.
Lattice parameter: Fig. 458.5a | Dielectric constant: Fig. 459.
Curie constant: Fig. 460.

6a | Transition heat: Fig. 461.

Nr. 1C-a11 $\text{BaTiO}_3\text{-PbTiO}_3$ 1b | Phase diagram: Fig. 462.
Lattice parameter: Fig. 463.

5a | Dielectric constant: Fig. 464.

6a | Specific heat: Fig. 465.
Transition heat: Fig. 466.

7 | Electromechanical properties: see 1A-8.

16 | Radiation damage: Fig. 467.

^{a)} Values in parentheses indicate that these values were assumed in order to determine α .

Nr. 1C-a12 $\text{CaZrO}_3\text{-BaZrO}_3$	1b Lattice parameter: Fig. 468.	Nr.
Nr. 1C-a13 $\text{CaZrO}_3\text{-PbZrO}_3$	1b Phase diagram: Fig. 469. 4 Thermal expansion: Fig. 470. 5a Dielectric constant: Fig. 471.	Nr.
Nr. 1C-a14 $\text{SrZrO}_3\text{-PbZrO}_3$	1b Phase diagram: Fig. 472, 473. Lattice parameter: Fig. 474. 4 Thermal expansion: Fig. 475, 476, 477; Tab. 64. 5a Dielectric constant: Fig. 478, 479. c Polarization: Fig. 480. 6a Specific heat: Fig. 481. Transition heat: Tab. 65.	Nr.
Tab. 64. PbZrO_3 , $(\text{Pb}_{0.95}\text{Sr}_{0.05})\text{ZrO}_3$, and $(\text{Pb}_{0.925}\text{Ba}_{0.075})\text{ZrO}_3$. $\Delta V/V$: anomalous volume change at the transition point. [54S2]		
Composition	$\Delta V/V [10^{-4}]$	
	Lowest phase	Intermediate phase
PbZrO_3	-41 at 230 °C	-
$(\text{Pb}_{0.925}\text{Ba}_{0.075})\text{ZrO}_3$	-43 at 150 °C	+24 at 190 °C
$(\text{Pb}_{0.95}\text{Sr}_{0.05})\text{ZrO}_3$	-30 at 210 °C	-20 at 230 °C
Tab. 65. PbZrO_3 , $(\text{Pb}_{0.95}\text{Sr}_{0.05})\text{ZrO}_3$, and $(\text{Pb}_{0.925}\text{Ba}_{0.075})\text{ZrO}_3$. ΔQ_m . [52S2]		
Composition	$\Delta Q_m [\text{cal mol}^{-1}]$	
	Lower transition	Upper transition
PbZrO_3	-	440
$(\text{Pb}_{0.925}\text{Ba}_{0.075})\text{ZrO}_3$	190	230
$(\text{Pb}_{0.95}\text{Sr}_{0.05})\text{ZrO}_3$	180	230
Nr. 1C-a15 $\text{BaZrO}_3\text{-PbZrO}_3$	1b Phase diagram: Fig. 482. Lattice parameter: Fig. 483. 4 Thermal expansion: Fig. 484. 5a Dielectric constant: Fig. 485 ... 488. c Coercive field: Fig. 489. 8 Elastic properties: Fig. 490.	Nr.
Nr. 1C-a16 $\text{CaHfO}_3\text{-PbHfO}_3$	1b Phase diagram: Fig. 491. 5a Dielectric constant: Fig. 492.	Nr.
Nr. 1C-a17 $\text{SrHfO}_3\text{-PbHfO}_3$	1b Phase diagram: Fig. 493. 5a Dielectric constant: Fig. 494.	Nr.
Nr. 1C-a18 $\text{BaHfO}_3\text{-PbHfO}_3$	1b Phase diagram: Fig. 495.	Nr.
Nr. 1C-a19 $\text{CaSnO}_3\text{-SrSnO}_3$	1b Lattice parameter: Fig. 496.	Nr.
Nr. 1C-a20 $\text{BaSnO}_3\text{-SrSnO}_3$	1b Lattice parameter: see Fig. 496.	Nr.
Nr. 1C-a21 $\text{BaSnO}_3\text{-PbO:SnO}_2$	1b Phase diagram: Fig. 497. 5a Dielectric constant: Fig. 498.	Nr.
Nr. 1C-a22 $\text{CaTiO}_3\text{-CaZrO}_3$	1b Lattice parameter: Fig. 499.	Nr.

Nr. 1C-a23 BaTiO₃-BaZrO₃	1b	Phase diagram: Fig. 500. Lattice parameter: Fig. 501.			
	2a	Phase diagram: Fig. 502.			
	5a	Dielectric constant: Fig. 503.			
	8a	Elastic property: Fig. 504			
Nr. 1C-a24 BaTiO₃-BaHfO₃	1b	Phase diagram: Fig. 505. Lattice parameter: Fig. 506.			
	5a	Dielectric constant: Fig. 507.			
Nr. 1C-a25 BaTiO₃-BaSnO₃	1b	Phase diagram: Fig. 508. See also	59I2		
	2a	Phase diagram: Fig. 509.			
	4	Thermal expansion: Fig. 510.			
	5a	Dielectric constant: Fig. 511.			
Nr. 1C-a26 BaTiO₃-BaUO₃	1b	Lattice parameter: Fig. 512.			
Nr. 1C-a27 PbTiO₃-PbZrO₃					
Pb(Zr _x Ti _{1-x})O ₃ with $x = 0.5 \dots 0.6$; for electromechanical properties of these very important piezoelectric materials, see 1C-a28.					
1a	Ferro- and antiferroelectric phase transitions in the PbTiO ₃ -PbZrO ₃ system were revealed in 1952 by SHIRANE, SUZUKI and TAKEDA.				
b	Phase diagram at high temperature: Fig. 513. Phase diagram: Fig. 514, 515. Lattice parameter: Fig. 516, 517.				
2	Flux method:				
4	Lattice distortion: Fig. 518a, b, 519. Thermal expansion: Fig. 520, 521, 522.				
5a	Dielectric constant: Fig. 523 ... 526.				
c	Spontaneous polarization: Fig. 527. Critical field: Fig. 528.				
6	Specific heat: Fig. 529, 530. Transition energy: Tab. 66.				
7	Electromechanical properties: see 1C-a28.				
8					
9	Birefringence: Fig. 531a, b, c.				
16	Radiation damage: Fig. 532.				
Tab. 66. Pb(Zr-Ti)O ₃ . Transition energy and entropy. [53S1]. x : atomic percent of PbTiO ₃ ; $d\Theta/dx$: shift of the transition temperature with x ; $dS(d\Theta/dx)$: it may be assumed that the free energy should decrease with the rate of $dS(d\Theta/dx)$ with increasing x .					
Kind of the phase change	Θ °C	ΔQ_m cal mol ⁻¹	ΔS_m cal mol ⁻¹ K ⁻¹	$d\Theta/dx$	$dS(d\Theta/dx)$
$A_\alpha \rightarrow P_\alpha$	230 > T > 225	400	0.8	—	(-5.8)
$A_\alpha \rightarrow A_\beta$	225	110	0.22	-16	-3.5
$A_\beta \rightarrow F_\alpha$	230	290	0.58	-4	-2.3
$A_\alpha \rightarrow F_\alpha$	240	—	—	-19	—
$F_\alpha \rightarrow P_\alpha$	217	250	0.51	+ 1.0	+ 0.5
$A_\beta \rightarrow F_\alpha$	—	40	0.08	—	—

Nr. 1C-a28 $\text{Pb}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$ ($x = 0.5 \dots 0.6$, lead zirconate-titanate)									
For general properties of $\text{PbTiO}_3\text{-PbZrO}_3$ see 1C-a27.									
1a	JAFFE, ROTH, and MARZULLO discovered the excellent piezoelectric performances of $\text{Pb}(\text{Zr-Ti})\text{O}_3$ ceramics in 1954. PZT is the trade mark of this substance developed by Clevite Corporation, Cleveland, Ohio, USA.								
5a	Dielectric constants: Fig. 533 and Fig. 539, 540, 541, 543, 544.								
7) 8)	Electromechanical properties (ceramics): Tab. 67; Fig. 534 ... 538; Tab. 68 ... 72; Fig. 539 ... 542; Tab. 73; Fig. 543 ... 554.								
10	Electrical conductivity: see For breakdown, see								
Tab. 67. $\text{Pb}(\text{Ti}_{1-x}\text{Zr}_x)\text{O}_3$ [$x = 0.48 \dots 0.60$] (ceramics). Electromechanical constants at RT. [60B3]									
Zr/Ti atom ratio	k_{31}	k_p	k_{15}	k_{33}	x_{11}^T	x_{11}^S	x_{33}^T	x_{33}^S obs	x_{33}^S calc
48/52	0.170	0.289	0.408	0.435	663	551	666	540	537
50/50	0.230	0.397	0.504	0.546	855	631	846	585	585
52/48	0.313	0.529	0.694	0.670	1180	612	730	399	389
54/46	0.280	0.470	0.701	0.626	990	504	450	253	268
56/44	0.267	0.450	0.657	0.619	840	477	423	246	258
58/42	0.254	0.428	0.646	0.607	751	437	397	243	246
60/40	0.238	0.400	0.625	0.585	672	410	376	240	245
	s_{11}^E	s_{11}^D	s_{33}^E	s_{33}^D	s_{44}^E	s_{44}^D	s_{66}	s_{12}^E	s_{12}^D
	$10^{-12} \text{ m}^2 \text{ N}^{-1}$								
48/52	10.8	10.5	10.9	8.83	28.3	23.6	28.3	-3.35	-3.66
50/50	12.4	11.7	13.3	9.35	32.8	24.5	32.9	-4.06	-4.72
52/48	13.8	12.4	17.1	9.35	48.2	25.0	38.4	-4.07	-5.38
54/46	11.6	10.7	14.8	9.0	45.0	22.9	29.9	-3.33	-4.24
56/44	11.0	10.2	14.0	8.65	39.8	22.6	28.4	-3.22	-4.01
58/42	10.5	9.85	12.8	8.10	37.7	21.9	27.1	-3.07	-3.75
60/40	10.4	9.75	12.05	7.92	36.9	22.5	26.7	-2.96	-3.55
	g_{31}	g_{33}	g_{15}	$g_{33} - g_{31}$	d_{31}	d_{33}	d_{15}	$d_{33} - d_{31}$	$\frac{s_{33}^D + s_{11}^D}{-2s_{13}^D}$
	$10^{-3} \text{ m}^2 \text{ C}^{-1}$				$10^{-12} \text{ C N}^{-1}$				$10^{-12} \text{ m}^2 \text{ N}^{-1}$
48/52	- 7.3	18.7	28.4	26.0	43.0	110	166	153	24.1
50/50	- 9.35	23.1	33.2	32.4	70.0	173	251	243	26.2
52/48	- 14.5	34.5	47.2	49.0	93.5	223	494	316	26.9
54/46	- 15.1	38.1	50.3	53.2	60.2	152	440	212	25.1
56/44	- 14.5	37.8	48.0	52.3	54.3	142	357	196	24.0
58/42	- 13.9	36.7	48.8	50.6	48.9	129	325	178	22.6
60/40	- 13.3	35.2	49.3	48.5	44.2	117	293	161	22.0
	Q_{mech}	Q_E (= 1/ $\tan \delta$)	P	c_{33}^D	$-s_{12}^E$	$-s_{12}^D$	$-s_{13}^E$	$-s_{13}^D$	$\sqrt{s_{33}^E s_{11}^E}$
			10^{-2} C m^{-2}	10^{10} N m^{-2}	s_{11}^E	s_{11}^D	$\sqrt{s_{33}^E s_{11}^E}$	$\sqrt{s_{33}^D s_{11}^D}$	$\sqrt{s_{33}^D s_{11}^D}$
48/52	1170	380	17	14.0	0.310	0.349	0.296	0.250	
50/50	950	370	27	13.5	0.328	0.404	0.329	0.249	
52/48	860	360	36	13.4	0.295	0.434	0.376	0.238	
54/46	680	300	42.5	14.8	0.288	0.396	0.380	0.273	
56/44	490	190	48	15.3	0.293	0.394	0.373	0.274	
58/42	500	200	43	15.8	0.292	0.381	0.355	0.261	
60/40	600	210	33	15.6	0.285	0.365	0.332	0.247	

Tab. 68. $(\text{Pb}_{1-x}\text{Sr}_x)(\text{Zr}_{1-y}\text{Ti}_y)\text{O}_3$ and $(\text{Pb}_{1-x}\text{Ca}_x)(\text{Zr}_{1-y}\text{Ti}_y)\text{O}_3$ (modified ceramics). Effects of Ca and Sr on electromechanical properties. [59K4]

Intended composition	ρ_a 10^3 kg m $^{-3}$	x at 1 kHz	24 hours after poling						Θ_t °C
			x at 1 kHz	$\tan \delta$ % at 1 kHz	k_p	d_{31} 10^{-12} CN $^{-1}$	g_{31} 10^{-3} m 2 C $^{-1}$	$(s_{11}^E)^{-1}$ 10^{10} Nm $^{-2}$	
$\text{Pb}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.40	736	544	0.5	0.48	71	14.7	7.67	385
$\text{Pb}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.39	707	542	0.4	0.47	69	14.4	7.76	
$\text{Pb}_{0.99}\text{Ca}_{0.01}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.42	729	624	0.5	0.49	77	13.9	7.89	
$\text{Pb}_{0.99}\text{Sr}_{0.01}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.42	755	584	0.6	0.49	75	14.5	7.68	
$\text{Pb}_{0.95}\text{Ca}_{0.05}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.26	832	973	0.5	0.44	88	10.2	7.62	
$\text{Pb}_{0.95}\text{Sr}_{0.05}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.47	920	1002	0.4	0.50	101	11.4	7.65	360
$\text{Pb}_{0.92}\text{Ca}_{0.08}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	6.86	794	888	0.4	0.32	60	7.6	7.85	
$\text{Pb}_{0.925}\text{Sr}_{0.075}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.29	942	1094	0.3	0.50	103	10.6	7.94	
$\text{Pb}_{0.90}\text{Sr}_{0.10}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.22	997	1129	0.3	0.49	103	10.3	7.95	290
$\text{Pb}_{0.875}\text{Sr}_{0.125}(\text{Zr}_{0.47}\text{Ti}_{0.53})\text{O}_3$	7.09	609	663	0.3	0.28	40	6.8	9.91	
$\text{Pb}_{0.875}\text{Sr}_{0.125}(\text{Zr}_{0.50}\text{Ti}_{0.50})\text{O}_3$	7.11	813	880	0.3	0.33	57	7.3	9.05	
$\text{Pb}_{0.875}\text{Sr}_{0.125}(\text{Zr}_{0.52}\text{Ti}_{0.48})\text{O}_3$	7.10	973	1149	0.3	0.44	91	9.0	8.32	
$\text{Pb}_{0.875}\text{Sr}_{0.125}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.14	1076	1237	0.4	0.47	100	9.1	8.06	265
$\text{Pb}_{0.875}\text{Sr}_{0.125}(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$	7.16	1095	1325	0.6	0.51	119	10.1	7.51	
$\text{Pb}_{0.875}\text{Sr}_{0.125}(\text{Zr}_{0.56}\text{Ti}_{0.44})\text{O}_3$	7.14	1105	1210	0.4	0.51	116	10.8	7.31	
$\text{Pb}_{0.875}\text{Sr}_{0.125}(\text{Zr}_{0.59}\text{Ti}_{0.41})\text{O}_3$	7.17	919	585	0.4	0.45	66	12.7	8.39	
$\text{Pb}_{0.85}\text{Sr}_{0.15}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	6.90	1106	1260	0.5	0.43	97	8.7	7.68	242
$\text{Pb}_{0.80}\text{Sr}_{0.20}(\text{Zr}_{0.50}\text{Ti}_{0.50})\text{O}_3$	6.56	941	970	0.6	0.29	56	6.5	8.11	
$\text{Pb}_{0.80}\text{Sr}_{0.20}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	6.48	1212	1257	0.5	0.34	86	7.8	7.05	
$\text{Pb}_{0.80}\text{Sr}_{0.20}(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$	6.36	1182	1341	0.8	0.35	91	7.7	6.18	
$\text{Pb}_{0.80}\text{Sr}_{0.20}(\text{Zr}_{0.55}\text{Ti}_{0.45})\text{O}_3$	6.36	1200	1337	0.8	0.34	86	7.3	6.42	
$\text{Pb}_{0.80}\text{Sr}_{0.20}(\text{Zr}_{0.56}\text{Ti}_{0.44})\text{O}_3$	6.35	1107	1113	0.7	0.35	81	8.2	6.50	

Tab. 69. $\text{Pb}(\text{Zr-Ti})\text{O}_3$ (ceramics, modified). Electromechanical properties of $\text{Pb}(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$ with five-valent additives. [59K5]. $f_R \cdot r$: radial frequency constant

Addition wt. %	ρ_a 10^3 kg m $^{-3}$	Before poling		24 hours after poling						Θ_t °C
		x at 1 kHz	$\tan \delta$ % at 1 kHz	x at 1 kHz	$\tan \delta$ % at 1 kHz	k_p	$f_R \cdot r$ Hz \cdot m	d_{31} 10^{-12} CN $^{-1}$	Q_{mech}	
None	7.41	707	0.3	537	0.4	0.49	1641	71		390
None	7.29	706	0.4	513	0.5	0.50	1687	69		387
0.1 Nb_2O_5	7.26	598	0.3	508	0.4	0.38	1643	54		
0.5 Nb_2O_5	6.96	732	2.1	790	2.0	0.46	1443	94		
0.8 Nb_2O_5	7.36	965	1.6	1166	1.5	0.48	1606	105		
1.0 Nb_2O_5	7.36	1064	1.8	1308	1.6	0.53	1563	126	61	361
1.0 Nb_2O_5	7.60	1055	2.2	1242	2.2	0.54	1538	125		
1.2 Nb_2O_5	7.34	1011	2.0	1167	1.7	0.48	1614	104	70	
1.4 Nb_2O_5	7.37	1057	2.2	1218	1.9	0.50	1584	113	69	
1.7 Nb_2O_5	7.39	1058	2.0	1218	1.8	0.47	1594	105		
2.0 Nb_2O_5	7.37	1074	2.1	1202	2.0	0.50	1550	115		344
0.5 Nb_2O_5	7.39	1169	2.1	1377	2.0	0.57	1491	146	48	369
0.5 La_2O_3	7.31	989	1.5	1187	1.5	0.49	1563	111	61	
1.0 Ta_2O_5	7.22	918	2.0	1121	2.1	0.50	1525	114		368
2.0 Ta_2O_5	7.49	1062	2.2	1230	2.1	0.50	1547	115		
2.0 Ta_2O_5	7.40	1077	1.8	1275	1.8	0.48	1581	111		364
2.5 Ta_2O_5	7.23	959	2.7	1112	2.4	0.36	1518	82	28	
5.0 Ta_2O_5	6.75	995	2.5	1052	2.6	0.33	1508	76		

Figuren S. 313ff.

II 1 Oxide des Perowskit-Typs

Tab. 70. $\text{Pb}(\text{Zr}-\text{Ti})\text{O}_3$ (ceramics, modified). Electromechanical properties of $\text{Pb}(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$ with three-valent additives. [59K5]. $f_R \cdot r$: radial frequency constant

Addition wt. %	ρ_a 10^3 kg m $^{-3}$	Before poling		24 hours after poling					Θ_f °C
		χ at 1 kHz	$\tan \delta$ % at 1 kHz	χ at 1 kHz	$\tan \delta$ % at 1 kHz	k_p	$f_R \cdot r$ Hz · m	d_{31} 10^{-12} CN $^{-1}$	
None	7.41	707	0.3	537	0.4	0.49	1641	71	390
None	7.29	706	0.4	513	0.5	0.50	1687	69	387
1.0 Y_2O_3	7.26	796	0.9	841	1.0	0.34	1547	66	374
1.0 La_2O_3	7.46	1187	1.9	1483	2.0	0.53	1510	138	
1.0 La_2O_3	7.47	1139	2.2	1387	2.1	0.52	1522	130	339
1.0 Nd_2O_3	7.43	1111	1.6	1395	1.8	0.49	1512	123	
1.0 Nd_2O_3	7.37	1101	1.9	1354	1.8	0.48	1511	119	348
1.0 didymia	7.41	1122	2.2	1341	2.2	0.50	1499	125	
2.0 La_2O_3	7.49	1296	2.6	1545	2.3	0.51	1545	132	
1.0 La_2O_3	7.20	1375	2.1	1792	1.7	0.51	1528	147	
1.0 Nd_2O_3	7.35	1362	2.2	1776	1.9	0.49	1558	136	
0.1 La_2O_3	6.75	790	0.4	870	0.6	0.42	1505	88	
0.2 La_2O_3	6.45	686	0.7	735	0.9	0.37	1419	78	
0.4 La_2O_3	6.44	942	1.4	1100	1.5	0.42	1407	109	
0.8 La_2O_3	7.19	1288	1.8	1682	1.8	0.49	1516	139	
1.0 La_2O_3	7.50	1255	2.4	1532	2.4	0.50	1550	128	

Tab. 71. Electromechanical properties of $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$ (ceramics), modified with additives of 1 wt% Nb. [59K5]. $f_R \cdot r$: radial frequency constant

Base composition	ρ_a 10^3 kg m $^{-3}$	Before poling		24 hours after poling					Q_{mech}
		χ at 1 kHz	$\tan \delta$ % at 1 kHz	χ at 1 kHz	$\tan \delta$ % at 1 kHz	k_p	$f_R \cdot r$ Hz · m	d_{31} 10^{-12} CN $^{-1}$	
$\text{Pb}(\text{Zr}_{0.50}\text{Ti}_{0.50})\text{O}_3$	7.38	879	1.5	1041	1.2	0.42	1696	82	81
$\text{Pb}(\text{Zr}_{0.51}\text{Ti}_{0.49})\text{O}_3$	7.31	975	1.6	1188	1.3	0.45	1642	97	73
$\text{Pb}(\text{Zr}_{0.52}\text{Ti}_{0.48})\text{O}_3$	7.39	985	1.5	1200	1.4	0.45	1640	97	76
$\text{Pb}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.43	1092	1.8	1371	1.4	0.53	1547	130	61
$\text{Pb}(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$	7.44	1051	1.8	1296	1.7	0.54	1549	128	62
$\text{Pb}(\text{Zr}_{0.55}\text{Ti}_{0.45})\text{O}_3$	7.40	955	2.4	973	2.0	0.56	1524	117	55
$\text{Pb}(\text{Zr}_{0.56}\text{Ti}_{0.44})\text{O}_3$	7.38	818	2.8	745	2.5	0.53	1601	93	56
$\text{Pb}(\text{Zr}_{0.57}\text{Ti}_{0.43})\text{O}_3$	7.41	750	3.0	684	2.5	0.50	1636	82	60
$\text{Pb}(\text{Zr}_{0.58}\text{Ti}_{0.42})\text{O}_3$	7.41	713	3.0	630	2.8	0.49	1676	75	62

Tab. 72. Electromechanical properties of $(\text{Pb}_{0.95}\text{Sr}_{0.05})(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$ (ceramics) with Nb_2O_5 or Ta_2O_5 . [59K5]. $f_R \cdot r$: radial frequency constant

Addition wt. %	ρ_a 10^3 kg m $^{-3}$	Before poling		24 hours after poling					Θ_f °C
		χ at 1 kHz	$\tan \delta$ % at 1 kHz	χ at 1 kHz	$\tan \delta$ % at 1 kHz	k_p	$f_R \cdot r$ Hz · m	d_{31} 10^{-12} CN $^{-1}$	
1.0 Nb_2O_5	7.34	1291	2.0	1609	2.0	0.56	1512	153	306
2.0 Nb_2O_5	7.22	1380	2.4	1662	2.1	0.47	1562	127	
3.0 Nb_2O_5	6.63	1125	2.1	1301	2.1	0.36	1550	91	
2.0 Ta_2O_5	7.33	1343	2.3	1695	2.0	0.54	1517	151	296

ith	
θ_f	°C
90	
87	
74	
339	
348	
% Nb.	
Q_{mech}	
81	
73	
76	
61	
62	
55	
56	
60	
62	
r Ta ₂ O ₅	
θ_f	°C
306	
296	

Tab. 73: PZT (commercial modified ceramics). Electromechanical constants at RT. [66b1]

Substance	x_{11}^T	x_{11}^S	x_{33}^T	x_{33}^S	d_{15}	d_{31}	d_{33}	e_{15}	e_{31}	e_{33}	ε_{15}	ε_{31}	ε_{33}	g_{31}	g_{33}	h_{15}	
					$10^{-12} \text{ C N}^{-1}$				C m^{-2}				$10^{-3} \text{ m}^2 \text{ C}^{-1}$				10^8 N C^{-1}
																$10^{-12} \text{ m}^2 \text{ N}^{-1}$	
PZT-2	990	504	450	260	440	-60.2	152	9.8	-1.86	9.0	50.3	-15.1	38.1	21.9			
	1475	730	1300	635	496	-123	289	12.7	-5.2	15.1	39.4	-11.1	26.1	19.7			
	1730	916	1700	830	584	-171	374	12.3	-5.4	15.8	38.2	-11.4	24.8	15.2			
	3130	1700	3400	1470	741	-274	593	17.0	-6.55	23.3	26.8	-9.11	19.7	11.3			
	PZT-4	PZT-5A	PZT-5H	PZT-6A	PZT-6B	PZT-7A	PZT-8										
	515	441	500	420	135	-29	76	4.8	-0.96	7.4	29.6	-6.6	17.3	12.2			
	840	450	425	235	368	-61	153	9.3	-2.15	9.7	49.5	-16.2	40.7	23.4			
	1000					-95	215					-10.5		24.5			
																$10^{-12} \text{ m}^2 \text{ N}^{-1}$	
				10^8 N C^{-1}													
																$10^{-12} \text{ m}^2 \text{ N}^{-1}$	
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Nr. 1C-a29 $\text{PbTiO}_3\text{-PbHfO}_3$	1b Phase diagram: Fig. 555, 556
Nr. 1C-a30 $\text{PbTiO}_3\text{-PbO:SnO}_2$	1b Phase diagram: Fig. 557. 5a Dielectric constant: Fig. 558.
Nr. 1C-a31 $\text{PbZrO}_3\text{-PbHfO}_3$	1b Phase diagram: Fig. 559.
Nr. 1C-a32 $\text{PbZrO}_3\text{-PbO:SnO}_2$	1b Phase diagram: Fig. 560. Lattice parameter: Fig. 561. 4 Thermal expansion: Fig. 562, 563. 5a Dielectric constant: Fig. 564a, b.
Nr. 1C-a33 $\text{LaFeO}_3\text{-BiFeO}_3$	1b Phase diagram: Fig. 565. Lattice parameter: Fig. 566a, b. 5a Dielectric constant: Fig. 567. 11 Magnetization: see Fig. 565.
Nr. 1C-b1 $\text{NaNbO}_3\text{-KTaO}_3$	1b Phase diagram: Fig. 568. Lattice parameter: Fig. 569. 4 Thermal expansion: Fig. 570. 5a Dielectric constant: Fig. 571.
Nr. 1C-b2 $\text{NaNbO}_3\text{-KSbO}_3$	1a Curie temperature: see Fig. 423.
Nr. 1C-b3 $\text{BaTiO}_3\text{-PbZrO}_3$	4 Thermal expansion: Fig. 572. 5a Dielectric constant: Fig. 573.
Nr. 1C-b4 $\text{BaTiO}_3\text{-PbO:SnO}_2$	1b Phase diagram: Fig. 574. 5a Dielectric constant: Fig. 575.
Nr. 1C-b5 $\text{PbTiO}_3\text{-CaZrO}_3$	1b Phase diagram: Fig. 576. Lattice parameter: Fig. 577. 5a Dielectric constant: Fig. 578.
Nr. 1C-b6 $\text{PbTiO}_3\text{-CaSnO}_3$	1b Phase diagram: see Fig. 576. Lattice parameter: Fig. 579. 5a Dielectric constant: Fig. 580.
Nr. 1C-b7 $\text{PbTiO}_3\text{-SrZrO}_3$	1b Phase diagram: Fig. 581. Lattice parameter: Fig. 582a, b. 5a Dielectric constant: Fig. 583.
Nr. 1C-b8 $\text{PbTiO}_3\text{-SrSnO}_3$	1b Phase diagram: Fig. 584. Lattice parameter: Fig. 585a, b. 5a Dielectric constant: Fig. 586.
Nr. 1C-b9 $\text{PbTiO}_3\text{-BaZrO}_3$	1b Phase diagram: Fig. 587. Lattice parameter: Fig. 588a, b. 5a Dielectric constant: Fig. 589. 7a Electromechanical property: Tab. 74.

Tab. 74. $(1 - x)\text{PbTiO}_3 - x\text{BaZrO}_3$ (ceramics). k_p and d_{33} at RT. [63B15]

x	Poling field $\cdot 10^5 \text{ V m}^{-1}$ [T in $^\circ\text{C}$]	k_p	d_{33} $\cdot 10^{-12} \text{ C N}^{-1}$
0.25	29 [185 ... 40]	0.16	40
0.30	27 [170 ... 40]	0.23	50
0.35	39 [145 ... 40]	0.30	110
0.40	30 [120 ... 40]	0.17	45

Nr. 1C-b10 $\text{PbTiO}_3\text{-BaSnO}_3$ 1b | Phase diagram: Fig. 590.
Lattice parameter: Fig. 591a, b.Nr. 1C-b11 $\text{LaAlO}_3\text{-BiFeO}_3$ 1b | Phase diagram: Fig. 592.
Lattice parameter: Fig. 593.
5a | Dielectric constant: Fig. 594.Nr. 1C-b12 $\text{LaCrO}_3\text{-BiFeO}_3$ 1b | Phase diagram: Fig. 595.
Lattice parameter: Fig. 596a, b.
4 | Thermal expansion: Fig. 597.
11 | Spontaneous magnetization: see Fig. 595.Nr. 1C-c1 $\text{NaNbO}_3\text{-CaTiO}_3$ 1b | Phase diagram: Fig. 598.
5a | Dielectric constant: Fig. 599.Nr. 1C-c2 $\text{NaNbO}_3\text{-BaTiO}_3$

1b | Phase diagram: Fig. 600.

Nr. 1C-c3 $\text{NaNbO}_3\text{-PbTiO}_3$ 1b | Transition temperature: Fig. 601.
5a | Dielectric constant: Fig. 602.Nr. 1C-c4 $\text{NaNbO}_3\text{-PbZrO}_3$ 1b | Phase diagram: Fig. 603.
5a | Dielectric constant: Fig. 604a, b.Nr. 1C-c5 $\text{KNbO}_3\text{-BaTiO}_3$ 1b | Phase diagram: Fig. 605.
Lattice parameter: Fig. 606.
5a | Dielectric constant: Fig. 607a, b, c.Nr. 1C-c6 $\text{KNbO}_3\text{-PbTiO}_3$ 1b | Phase diagram: Fig. 608.
Lattice parameter: Fig. 609.
5a | Dielectric constant: Fig. 610a, b.Nr. 1C-c7 $\text{SrTiO}_3\text{-BiFeO}_3$ 1b | Phase diagram: Fig. 611.
Lattice parameter: Fig. 612.
5a | Relaxation phenomena are observed in the range II [65F1].Nr. 1C-c8 $\text{BaTiO}_3\text{-LaAlO}_3$

1b | Lattice parameter and Curie temperature: Tab. 75.

Tab. 75. $\text{BaTiO}_3\text{-LaAlO}_3$. Lattice parameters and θ_f . [5814]

Concentration mol%		<i>a</i> Å	<i>c</i> Å	<i>c/a</i>	<i>V</i> Å ³	θ_f °C
BaTiO ₃	LaAlO ₃					
100.0	—	3.9956	4.0352	1.0100	64.42	+120
99.0	1.0	3.9951	4.0345	1.0098	64.39	+87
97.5	2.5	3.9949	4.0293	1.0086	64.30	+46
95.0	5.0	4.0050	—	1.0000	64.24	-14
92.5	7.5	4.0011	—	1.0000	64.05	-85
90.0	10.0	3.9984	—	1.0000	63.92	-133
87.5	12.5	3.9950	—	1.0000	63.76	—
85.0	15.0	3.9906	—	1.0000	63.55	—
75.0	25.0	3.9800	—	1.0000	63.04	—
—	100.0	3.7950	—	1.0000	54.65	—

Nr. 1C-c9 $\text{BaTiO}_3\text{-BiFeO}_3$ 11 | Néel temperature and magnetic resonance line width:
12 | Fig. 613.Nr. 1C-c10 $\text{PbTiO}_3\text{-LaAlO}_3$ 1b | Phase diagram: Fig. 614.
Lattice parameter: Fig. 615.
5a | Dielectric constant: Fig. 616.Nr. 1C-c11 $\text{PbTiO}_3\text{-LaMnO}_3$ 1b | Transition temperatures: Fig. 617.
Lattice parameters: Fig. 618.Nr. 1C-c12 $\text{PbTiO}_3\text{-LaFeO}_3$ 1b | Phase diagram: Fig. 619.
Lattice parameter: Fig. 620.
5a | Dielectric constant: Fig. 621.Nr. 1C-c13 $\text{PbTiO}_3\text{-BiFeO}_3$ 1b | Phase diagram: Fig. 622a, b.
Lattice parameter: Fig. 623a, b.
4 | Thermal expansion: Fig. 624.
5a | Dielectric constant: Fig. 625.Nr. 1C-c14 $\text{PbZrO}_3\text{-BiFeO}_3$ 1b | Phase diagram: Fig. 626.
Lattice parameter: Fig. 627.
5a | Dielectric constant: Fig. 628.Nr. 1C-c15 $\text{SrSnO}_3\text{-BiFeO}_3$ 1b | Phase diagram: Fig. 629.
12c | Mössbauer absorption: Fig. 630.Nr. 1C-c16 $\text{SrFeO}_3\text{-BiFeO}_3$ 1a | Unit cell volume: Fig. 631.
11 | Magnetization: Fig. 632.Nr. 1C-d1 $\text{SrTiO}_3\text{-Sr(Fe}_{1/2}\text{Ta}_{1/2}\text{)O}_3$

1b | Phase diagram: Fig. 633.

Nr. 1C-d2 $\text{BaTiO}_3\text{-Ba(Fe}_{1/2}\text{Ta}_{1/2}\text{)O}_3$

2b | Phase diagram: Fig. 634.

Nr. 1C-d3 $\text{BaTiO}_3\text{-(K}_{1/2}\text{Bi}_{1/2}\text{)TiO}_3$ 1b | Curie temperature: Fig. 635.
Lattice parameters: Fig. 636.Nr. 1C-d4 $\text{PbTiO}_3\text{-(Na}_{1/2}\text{Bi}_{1/2}\text{)TiO}_3$ 1b | Phase diagram and lattice parameters: Fig. 637.
5a | Dielectric constant: Fig. 638.Nr. 1C-d5 $\text{PbTiO}_3\text{-(K}_{1/2}\text{Bi}_{1/2}\text{)TiO}_3$

1b | Curie temperature and lattice parameters: Fig. 639.

Nr. 1C-d6 $\text{PbTiO}_3\text{-(Li}_{1/2}\text{La}_{1/2}\text{)TiO}_3$

1b | Curie temperature and lattice parameters: Fig. 640.

Nr. 1C-d7 $\text{PbTiO}_3\text{-}(\text{Na}_{1/2}\text{La}_{1/2})\text{TiO}_3$	1b Curie temperature and lattice parameters: Fig. 641.			
Nr. 1C-d8 $\text{PbTiO}_3\text{-}(\text{Li}_{1/2}\text{Ce}_{1/2})\text{TiO}_3$	1b Lattice parameters: Fig. 642.			
Nr. 1C-d9 $\text{PbTiO}_3\text{-}(\text{Li}_{1/2}\text{Nd}_{1/2})\text{TiO}_3$	1b Lattice parameters: Fig. 643.			
Nr. 1C-d10 $\text{PbTiO}_3\text{-Pb}(\text{Mg}_{1/2}\text{W}_{1/2})\text{O}_3$	1b Phase diagram: Fig. 644. Lattice parameters: Fig. 645.			
Nr. 1C-d11 $\text{PbTiO}_3\text{-Pb}(\text{Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$	1b Curie temperature: Fig. 646.			
Nr. 1C-d12 $\text{PbTiO}_3\text{-Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b Curie temperature: Fig. 647.			
Nr. 1C-d13 $\text{PbTiO}_3\text{-Pb}(\text{Mn}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b Transition temperature: Fig. 648. Lattice parameters: Fig. 649.			
Nr. 1C-d14 $\text{PbZrO}_3\text{-Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b Curie temperature: see Fig. 647.			
Nr. 1C-d15 $\text{PbZrO}_3\text{-Pb}(\text{Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$	1b Curie temperature: Fig. 650.			
Nr. 1C-d16 $\text{PbZrO}_3\text{-}(\text{Na}_{1/2}\text{Bi}_{1/2})\text{ZrO}_3$	1b Phase diagram: Fig. 651. 4 Lattice distortion: Fig. 652. 5a Dielectric constant: Fig. 653.			
Nr. 1C-d17 $\text{PbZrO}_3\text{-}(\text{K}_{1/2}\text{Bi}_{1/2})\text{ZrO}_3$	1b Phase diagram: Fig. 654. Lattice parameters: Tab. 76. 4 Lattice distortion: Fig. 655. 5a Dielectric constants: Fig. 656.			
Tab. 76. $(1 - x)\text{PbZrO}_3 - x(\text{K}_{1/2}\text{Bi}_{1/2})\text{ZrO}_3$. Lattice constants at RT [62B10]				
x	a Å	b Å	c Å	
0	5.884	11.768	8.220	orthorhombic
0.10	5.882	11.764	8.227	orthorhombic
0.20	5.877	11.755	8.237	orthorhombic
0.30	5.876	11.751	8.248	orthorhombic
0.40	4.151	—	—	cubic
0.50	4.152	—	—	cubic
Nr. 1C-d18 $\text{PbHfO}_3\text{-Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b Curie temperature: see Fig. 647.			
Nr. 1C-d19 $\text{Pb}(\text{Mg}_{1/2}\text{W}_{1/2})\text{O}_3\text{-Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$	1b Phase diagram: Fig. 657.			
Nr. 1C-d20 $(\text{Na}_{1/2}\text{Bi}_{1/2})\text{TiO}_3\text{-}(\text{K}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$	1b Curie temperature: see Fig. 635. Lattice parameters: see Fig. 636.			
Nr. 1C-d21 $\text{PbZrO}_3\text{-}(\text{Na}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$	1b Phase diagram: Fig. 658. Lattice parameters: Fig. 659.			
Nr. 1C-d22 $\text{BiFeO}_3\text{-Sr}(\text{Sn}_{1/3}\text{Mn}_{2/3})\text{O}_3$	1b Phase diagram: Fig. 660. Lattice parameters: Fig. 661. 12c Mössbauer effect: see [65M8]			
Nr. 1C-d23 $\text{BiFeO}_3\text{-Pb}(\text{Fe}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b Lattice parameters: Fig. 662. 5a Dielectric constant: Fig. 663. 11 Magnetic susceptibility: Fig. 664. Néel temperature and spontaneous magnetization: Fig. 665.			

Nr. 1C-e1 $\text{NaNbO}_3\text{-LiNbO}_3$	1b Phase diagram: Fig. 666. 5a Dielectric constant: Fig. 667.										
Nr. 1C-e2 $\text{NaNbO}_3\text{-NaVO}_3$	5a Dielectric constant: Fig. 668. 14b Switching: see Fig. 9.										
Nr. 1C-e3 $\text{NaNbO}_3\text{-CaNb}_2\text{O}_6$	1b Phase diagram: Fig. 669. 5a Dielectric constant: Fig. 670.										
Nr. 1C-e4 $\text{NaNbO}_3\text{-CdNb}_2\text{O}_6$	1b Phase diagram: Fig. 671, 672. Lattice parameter: Fig. 673. 5a Dielectric constant: Fig. 674; Tab. 77. 7a Piezoelectricity: Fig. 675; Tab. 78.										
Tab. 77. $(1 - x)\text{NaNbO}_3 - (x/2)\text{CdNb}_2\text{O}_6$ [56L2]. r : capacitance ratio; C : Curie constant; Θ_f , Θ compare Fig. 671, 672											
Composition x	Firing conditions			x_{RT}	r	Θ °C	x_{max}	Θ_f °C	$C \cdot 10^4$ °C	Θ_p °C	ρ 10^3 kg m^{-3}
	T °C	t hr	atmosphere								
0.02	1250	1	CdO	230	—	200	2700	375	12	345	3.9
0.05	1250	1	CdO	500	1200	60	4000	375	12	345	4.2
0.10	1250	1	CdO	1000	130	75	4100	320	18	275	4.3
0.15	1250	1	CdO	1400	40	50	8500	285	24	260	4.3
0.20	1250	1	CdO	2300	20	20	10000	250	14	250	4.4
0.25	1250	1	CdO	3500	10	5	15000	220	20	230	4.5
0.30	1220	2	CdO	2700	12	-25	11000	210	20	205	4.6
Tab. 78. $(1 - x)\text{NaNbO}_3 - (x/2)\text{CdNb}_2\text{O}_6$ (ceramics) [62K4]											
x	0.05	0.10	0.15	0.20	0.25	0.30					
ρ	4.2	4.3	4.3	4.3	4.4	4.2	10^3 kg m^{-3}				
$f_R \cdot 2r$	3.0	3.0	3.0	3.15	3.36	3.25	10^3 Hz m				
s_{11}^E	11.9	11.6	11.6	10.5	9.0	10.1	$10^{-12} \text{ m}^2 \text{ N}^{-1}$				
$\tan \delta$	0.01	0.01	0.02	0.01	0.01	0.03					
x at Θ_f	4	4.1	8.5	16	13	11	10^3				
Nr. 1C-e5 $\text{NaNbO}_3\text{-SrNb}_2\text{O}_6$	1b Phase diagram: Fig. 676. Lattice parameter: Fig. 677. 5a Dielectric constant: Fig. 678. 7a Electromechanical properties: Fig. 679, 680, 681.										
Nr. 1C-e6 $\text{NaNbO}_3\text{-PbNb}_2\text{O}_6$	1b Phase diagram: Fig. 682. Lattice parameter: Fig. 683. 7a Electromechanical properties: Fig. 684.										
Nr. 1C-e7 $\text{CdTiO}_3\text{-LiNbO}_3$, $\text{CdTiO}_3\text{-LiTaO}_3$	5a Dielectric constant: Fig. 685.										
Nr. 1C-e8 $\text{SrTiO}_3\text{-Bi}_2\text{O}_3 \cdot 3\text{TiO}_2$	1b Lattice parameter: Fig. 686. 5a Dielectric constant: Fig. 687, 688.										
Nr. 1C-e9 $\text{BaTiO}_3\text{-BaNb}_2\text{O}_6$	1b Phase diagram: Fig. 689.										

Nr. 1C-e10 $\text{BaTiO}_3\text{-BaTa}_2\text{O}_6$	1b Lattice parameter: Fig. 690. 5a Dielectric constant: Fig. 691.
Nr. 1C-e11 $\text{BaTiO}_3\text{-A}_2\text{B}_2\text{O}_7$	1b Curie temperature: Fig. 692. 5a Dielectric constant: Fig. 693 ... 697.
Nr. 1C-e12 $\text{PbZrO}_3\text{-PbNb}_2\text{O}_6$	
For the solid solution with PbNb_2O_6 as an end material see 5B-8.	
	1b Phase diagram: Fig. 698. 4 Thermal expansion: Fig. 699. 5 Dielectric constant: Fig. 700.
Nr. 1C-e13 $\text{PbZrO}_3\text{-PbTa}_2\text{O}_6$	1b Phase diagram: Fig. 701. 4 Thermal expansion: see Fig. 699. 5 Dielectric constant: Fig. 702.
Nr. 1C-f1 $\text{CaTiO}_3\text{-SrTiO}_3\text{-BaTiO}_3$	1b Phase diagram: Fig. 703.
Nr. 1C-f2 $\text{CaTiO}_3\text{-BaTiO}_3\text{-PbTiO}_3$	1b Phase diagram: Fig. 704, 705. Curie temperature: Fig. 706. 7a Electromechanical properties: see Nr. 1A-8, 7a.
Nr. 1C-f3 $\text{PbTiO}_3\text{-PbZrO}_3\text{-PbO:SnO}_2$	1b Phase diagram: Fig. 707. 8b Elastic properties: Fig. 708, 709.
Nr. 1C-f4 $\text{PbTiO}_3\text{-PbHfO}_3\text{-PbO:SnO}_2$	1b Phase diagram: Fig. 710.
Nr. 1C-f5 $\text{PbTiO}_3\text{-PbZrO}_3\text{-LaFeO}_3$	1b Phase diagram: Fig. 711. Lattice parameters: Fig. 712.
Nr. 1C-f6 $\text{PbTiO}_3\text{-PbZrO}_3\text{-BiFeO}_3$	1b Phase diagram: Fig. 713. Lattice parameters: Fig. 714.
Nr. 1C-f7 $\text{PbTiO}_3\text{-PbZrO}_3\text{-Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$	1b Phase diagram: Fig. 715. Lattice parameters: Fig. 716. 7a Electromechanical property: Fig. 717, 718.
Nr. 1C-f8 $\text{PbTiO}_3\text{-PbZrO}_3\text{-Pb}(\text{Fe}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b Lattice parameters: Fig. 719. Curie temperature: Fig. 720. 7a Electromechanical property: Fig. 721.
Nr. 1C-f9 $\text{PbTiO}_3\text{-PbZrO}_3\text{-ABO}_3$	1b Phase diagram: Fig. 722.
Nr. 1C-f10 $\text{PbTiO}_3\text{-SrTiO}_3\text{-LaMnO}_3$	1b Curie temperature: Fig. 723.
Nr. 1C-f11 $\text{PbTiO}_3\text{-LaMnO}_3\text{-LaMeO}_3$ (Me = Fe, Co, Ni, Cr)	
	1b Transition temperatures: Fig. 724. 5a Dielectric constant: Fig. 725. 11 Magnetic susceptibility: see Fig. 725. Magnetization: Fig. 726.

Figuren S. 349 ff.

II 2 WO_3

Nr. 1C-f12 $\text{BaTiO}_3\text{-SrTiO}_3\text{-LaYO}_3\text{-LaInO}_3$	1b Phase diagram: Fig. 727.
Nr. 1C-f13 $\text{CaSnO}_3\text{-SrSnO}_3\text{-BaSnO}_3$	1b Phase diagram: Fig. 728.
Nr. 1C-f14 $(\text{Na-K})(\text{Nb-Ta})\text{O}_3$	1b Phase diagram: Fig. 729.
Nr. 1C-f15 $(\text{Ca-Ba})(\text{Ti-Zr})\text{O}_3$	1b Phase diagram: Fig. 730.
Nr. 1C-f16 $(\text{Sr-Pb})(\text{Ti-Zr})\text{O}_3$	1b Phase diagram: Fig. 731. Lattice parameter: Fig. 732. Transition temperature: Fig. 733.
Nr. 1C-f17 $(\text{Ba-Pb})(\text{Ti-Zr})\text{O}_3$	5a Dielectric constant: Fig. 734, 735.
Nr. 1C-f18 $(\text{Ba-Pb})(\text{Ti-Sn})\text{O}_3$	1b Phase diagram: Fig. 736. Lattice parameter: Fig. 737. Transition temperature: Fig. 738.
Nr. 1C-f19 $\text{BaTiO}_3\text{-PbTiO}_3\text{-BaNb}_2\text{O}_6\text{-PbNb}_2\text{O}_6$	7a Electromechanical properties: Fig. 739, 740.
	1b Phase diagram: Fig. 741, 742. Lattice parameter: Fig. 743. Transition temperature: Fig. 744.
	1b Phase diagram: Fig. 745. Lattice parameter: Fig. 746.

2 WO_3

2A Pure compound

Nr. 2A-1 WO_3 , Tungsten trioxide

1a	The anomalous dielectric properties of ceramic specimens of WO_3 were discovered by OGAWA ^{a)} in 1948. Possibility of ferroelectricity in WO_3 was pointed out by MATTIAS ^{b)} in 1949.								^{a)} 48N1, 48N2 ^{b)} 49M2
b	phase	VII	VI	V	IV	III	II	I	^{a)} 49M2
	state	F ^{a)}							^{b)} 60T1
	crystal system	mono-clinic ^{*b)}	tri-clinic ^{b)}	mono-clinic ^{c)}	ortho-rhombic ^{b)}	tetragonal ^{d)}	tetragonal ^{b)}	tetragonal ^{b)}	^{c)} 60T2
	space group			P2 ₁ /n ^{e)} -C _{2h}		P4/nmm ^{d)} -D _{4h}			^{d)} 52K1
	Θ	-40 ^{b)}	17 ^{b)}	330 ^{e)}	740 ^{e)}	910 ^{e)}	1230 ^{e)}	°C	^{e)} 56S1
	$T_{\text{melt}} = 1473$ °C. $\epsilon = 7.157 \cdot 10^3$ kg m ⁻³ at RT. $a = 7.30$ Å, $b = 7.53$ Å, $c = 7.68$ Å, $\beta = 90^\circ 54'$ at 30 °C. Transparent, bluish green.								21J1 04S1 60T1
2a	Crystal growth: Sublimation method.								51U1, 56T2, 59S3
b	Crystal form: Plate-like.								
3	Crystal structure: Fig. 747, 748; Tab. 79; Fig. 749.								60T1
	phase	VII	VI	V	IV	III	II	I	
	Z	4	8	8					
4	Lattice distortion: Tab. 80. Thermal expansion: Fig. 750 ... 754.								
5a	Dielectric constant: $\kappa = 100 \dots 300$ at liquid air temperature. No reliable dielectric measurements could be carried out at and above room temperature because of high electrical conductivity. $d\Theta_{\text{IV-III}}/dP = -8.46 \cdot 10^{-8}$ °K N ⁻¹ m ² .								49M2
c	Dielectric hysteresis loop was observed at liquid air temperature.								66T4 49M2

* As to the crystal system in the phase VII, possibility of triclinic symmetry was discussed by TANISAKI [60T1].

6a
9a

10
12c

14a

17

Tab.

W
W
O
O
O
O
O
O

3 L
3A

Nr. 1

1a
b

V Index of substances — Substanzenverzeichnis

This index consists of two parts: part A is for pure compounds (including complex compounds such as $Pb(Co_{1/2}Nb_{1/2})O_3$ or $Na_{0.5}Bi_{4.5}Ti_4O_{15}$) and part B is for solid solutions.

V A: In the 1st column the substances are ordered according to the alphabetically arranged gross formula. When their names (e.g. Rochelle salt) and/or their abbreviated names (e.g. TGS) are widely used, they are also included in this column. In the gross formula the numbers of the elements are determined by simple addition.

Compounds containing water of crystallization are, however, listed twice: (1) H and O of the water molecules are included in the gross formula, (2) the water molecules are attached separately to the gross formula. For instance, Rochelle salt is listed in the 1st column as $C_4H_4KNaO_6 \cdot 4H_2O$, $C_4H_{12}KNaO_{10}$ and also as Rochelle salt, RS, Seignette salt.

Crystals in which H is replaced by D (e.g. KD_2PO_4) are not listed separately, since data on their properties are presented in the same section as the data on the non-deuterated crystals (e.g. KH_2PO_4).

V B: In the 1st column the gross formula of each end material of a solid solution (e.g. $BaTiO_3$ or $PbTiO_3$ for the solid solution $BaTiO_3-PbTiO_3$) is listed in the same manner as in the case of pure compounds. Thus the solid solution $BaTiO_3-PbTiO_3$ can be found in the 2nd column by looking first for either BaO_3 Ti or O_3PbTi in the 1st column of Part B. If the solid solution is expressed by the formula such as $(Sb_xBi_{1-x})SI$, the end material can be obtained by putting x equal to either 0 or 1. When solid solutions have abbreviated names (e.g. KTN), these are also included in the 1st column.

Since in general one section corresponds to one substance in this volume, the 3rd column gives the section number and the 4th column gives the first page of the section.

Dieses Verzeichnis besteht aus zwei Teilen: Teil A enthält die reinen Verbindungen (einschließlich komplexer Verbindungen wie $Pb(Co_{1/2}Nb_{1/2})O_3$ oder $Na_{0.5}Bi_{4.5}Ti_4O_{15}$) und Teil B enthält die Mischkristalle.

V A: In der 1. Spalte sind die Substanzen nach der alphabetisch angeordneten Bruttoformel aufgeführt. Wenn ihre Namen (z. B. Seignette-Salz) und/oder ihre abgekürzten Bezeichnungen (z. B. TGS) häufig gebraucht werden, sind auch sie in dieser Spalte zu finden. In der Bruttoformel ist die Anzahl jedes Elements durch einfache Addition bestimmt.

Verbindungen, die Kristallwasser enthalten, sind zweimal aufgeführt: 1. H und O der Wassermoleküle sind in der Bruttoformel enthalten. 2. die Wassermoleküle werden getrennt der Bruttoformel hinzugefügt (z. B. Seignette-Salz ist in der 1. Spalte aufgeführt als $C_4H_4KNaO_6 \cdot 4H_2O$, $C_4H_{12}KNaO_{10}$ und auch als Rochelle-Salz, RS, Seignette-Salz).

Kristalle, in denen H durch D ersetzt ist (z. B. KD_2PO_4), werden nicht gesondert aufgeführt. Daten von ihren Eigenschaften erscheinen in demselben Abschnitt an der gleichen Stelle wie die Daten von den nicht deuterierten Kristallen (z. B. KH_2PO_4).

V B: In der 1. Spalte ist die Bruttoformel jeder Endsubstanz einer Mischkristallreihe (z. B. $BaTiO_3$ oder $PbTiO_3$ für die Mischkristallreihe $BaTiO_3-PbTiO_3$) in derselben Weise aufgeführt wie im Fall von reinen Verbindungen. So kann die Mischkristallreihe $BaTiO_3-PbTiO_3$ in der zweiten Spalte gefunden werden, wenn man zunächst entweder BaO_3 Ti oder O_3PbTi in der ersten Spalte von Teil B sucht. Wenn die Mischkristallreihe durch die Formel $(Sb_xBi_{1-x})SI$ ausgedrückt wird, kann man die Endsubstanz finden, indem man x gleich 0 oder 1 setzt. Wenn Mischkristalle abgekürzte Namen haben (z. B. KTN), sind diese auch in der 1. Spalte enthalten.

Da in diesem Band jeweils ein Abschnitt einer Substanz entspricht, gibt die 3. Spalte die Abschnittsnummer und die 4. Spalte die erste Seite des Abschnitts an.

VA Pure compounds

Gross formula	Chemical formula	Nr.	Page
ADP			
$AgC_2H_5N_2O_5$	$NH_4H_2PO_4$	13A-7	143
$Ag_2H_3IO_6$	$NH_2CH_2COOH \cdot AgNO_3$	29A-1	191
$AgNbO_3$	$Ag_2H_3IO_6$	35-22	209
AgO_3Ta	$AgNbO_3$	35-16	207
AgO_3V	$AgTaO_3$	35-18	207
$AlCH_3NO_8S_2 \cdot 12H_2O$	$AgVO_3$	35-20	208
$AlCH_5N_3O_8S_2 \cdot 6H_2O$	$CH_3NH_3Al(SO_4)_2 \cdot 12H_2O$	18A-4	158
$AlCH_{18}N_3O_{14}S_2$	$C(NH_2)_3Al(SO_4)_2 \cdot 6H_2O$	19A-1	161
$AlCH_{30}NO_{20}S_2$	$C(NH_2)_3Al(SO_4)_2 \cdot 6H_2O$	19A-1	161
$AlCH_6NO_8Se_2 \cdot 12H_2O$	$CH_3NH_3Al(SO_4)_2 \cdot 12H_2O$	18A-4	158
$AlCH_6N_3O_8Se_2 \cdot 6H_2O$	$CH_3NH_3Al(SeO_4)_2 \cdot 12H_2O$	18A-10	161
$AlCH_{18}N_3O_{14}Se_2$	$C(NH_2)_3Al(SeO_4)_2 \cdot 6H_2O$	19A-5	166
$AlCH_{30}NO_{20}Se_2$	$C(NH_2)_3Al(SeO_4)_2 \cdot 6H_2O$	19A-5	166
Ammonium metaphosphate	$CH_3NH_3Al(SeO_4)_2 \cdot 12H_2O$	18A-10	161
$AsCsH_2O_4$		35-14	205
AsH_2KO_4	CsH_2AsO_4	13A-6	143
	KH_2AsO_4	13A-4	141

V Substanzenverzeichnis

Gross formula	Chemical formula	Nr.	Page
AsH ₆ NO ₄	NH ₄ H ₂ AsO ₄	13A-8	147
AsH ₂ O ₄ Rb	RbH ₂ AsO ₄	13A-5	143
Azobenzene	C ₁₂ H ₁₀ N ₂	37-5	216
Azoxybenzene	C ₁₂ H ₁₀ N ₂ O	37-6	216
B ₂ BrCd ₃ O ₁₃	Cd ₃ B ₂ O ₁₃ Br	9A-18	120
B ₂ BrCo ₃ O ₁₃	Co ₃ B ₂ O ₁₃ Br	9A-14	119
B ₂ BrCr ₃ O ₁₃	Cr ₃ B ₂ O ₁₃ Br	9A-11	118
B ₂ BrCu ₃ O ₁₃	Cu ₃ B ₂ O ₁₃ Br	9A-16	119
B ₂ BrFe ₃ O ₁₃	Fe ₃ B ₂ O ₁₃ Br	9A-13	119
B ₂ BrMg ₃ O ₁₃	Mg ₃ B ₂ O ₁₃ Br	9A-10	118
B ₂ BrMn ₃ O ₁₃	Mn ₃ B ₂ O ₁₃ Br	9A-12	119
B ₂ BrNi ₃ O ₁₃	Ni ₃ B ₂ O ₁₃ Br	9A-15	119
B ₂ BrO ₁₃ Zn ₃	Zn ₃ B ₂ O ₁₃ Br	9A-17	120
B ₆ Ca ₂ H ₁₀ O ₁₆	Ca ₂ B ₆ O ₁₁ · 5H ₂ O	21A-1	173
B ₆ Ca ₂ O ₁₁ · 5H ₂ O	Ca ₂ B ₆ O ₁₁ · 5H ₂ O	21A-1	173
B ₇ Cd ₄ ClO ₁₃	Cd ₃ B ₇ O ₁₃ Cl	9A-9	118
B ₇ Cd ₃ IO ₁₃	Cd ₃ B ₇ O ₁₃ I	9A-25	122
B ₇ ClCo ₃ O ₁₃	Co ₃ B ₇ O ₁₃ Cl	9A-5	117
B ₇ ClCr ₃ O ₁₃	Cr ₃ B ₇ O ₁₃ Cl	9A-2	116
B ₇ ClCu ₃ O ₁₃	Cu ₃ B ₇ O ₁₃ Cl	9A-7	118
B ₇ ClFe ₃ O ₁₃	Fe ₃ B ₇ O ₁₃ Cl	9A-4	117
B ₇ ClMg ₃ O ₁₃	Mg ₃ B ₇ O ₁₃ Cl	9A-1	115
B ₇ ClMn ₃ O ₁₃	Mn ₃ B ₇ O ₁₃ Cl	9A-3	117
B ₇ ClNi ₃ O ₁₃	Ni ₃ B ₇ O ₁₃ Cl	9A-6	117
B ₇ ClO ₁₃ Zn ₃	Zn ₃ B ₇ O ₁₃ Cl	9A-8	118
B ₇ Co ₃ IO ₁₃	Co ₃ B ₇ O ₁₃ I	9A-22	121
B ₇ Cr ₃ IO ₁₃	Cr ₃ B ₇ O ₁₃ I	9A-19	120
B ₇ Fe ₃ IO ₁₃	Fe ₃ B ₇ O ₁₃ I	9A-21	120
B ₇ IMn ₃ O ₁₃	Mn ₃ B ₇ O ₁₃ I	9A-20	120
B ₇ INi ₃ O ₁₃	Ni ₃ B ₇ O ₁₃ I	9A-23	121
B ₇ IO ₁₃ Zn ₃	Zn ₃ B ₇ O ₁₃ I	9A-24	121
Ba ₄ Bi ₂ Fe ₂ Nb ₈ O ₃₀	Ba ₄ Bi ₂ Fe ₂ Nb ₈ O ₃₀	5C-g1	104
BaBi ₂ Nb ₂ O ₉	BaBi ₂ Nb ₂ O ₉	7A-7	109
BaBi ₃ NbO ₁₂ Ti ₂	BaBi ₃ Ti ₂ NbO ₁₂	7A-12	110
BaBi ₂ O ₉ Ta ₂	BaBi ₂ Ta ₂ O ₉	7A-8	109
BaBi ₄ O ₁₅ Ti ₄	BaBi ₄ Ti ₄ O ₁₅	7A-14	111
Ba ₂ Bi ₄ O ₁₈ Ti ₅	Ba ₂ Bi ₄ Ti ₅ O ₁₈	7A-19	112
BaC ₁₈ Ca ₂ H ₃₀ O ₁₂	Ca ₂ Ba(CH ₃ CH ₂ COO) ₆	26A-3	184
Ba ₄ Ce ₂ Nb ₈ Ni ₂ O ₃₀	Ba ₄ Ce ₂ Ni ₂ Nb ₈ O ₃₀	5C-d1	104
Ba ₄ Fe ₂ Gd ₂ Nb ₈ O ₃₀	Ba ₄ Gd ₂ Fe ₂ NbO ₃₀	5C-g4	104
Ba ₂ Fe ₃ Nb ₂ Nd ₄ O ₃₀	Ba ₂ Nd ₄ Fe ₃ Nb ₂ O ₃₀	5C-h1	104
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134	LiNbO ₃	NaNH ₄ SO ₄ · 2H ₂ O	17A-1	157
212	Li _{1/4} Nb _{1/4} O ₃ PbW _{1/2}	LiNbO ₃	3A-1	89
212	LiO ₃ Ta	Pb(Li _{1/4} Nb _{1/4} W _{1/2})O ₃	1B3-xvii	70
	LuMnO ₃	LiTaO ₃	3A-2	92
95	Lu _{1/2} Nb _{1/2} O ₃ Pb	LuMnO ₃	4A-6	97
200	Lu _{1/2} O ₃ PbTa _{1/2}	Pb(Lu _{1/2} Nb _{1/2})O ₃	1B3-ix	68
	MASD	Pb(Lu _{1/2} Ta _{1/2})O ₃	1B3-xv	70
210	Mg _{1/4} Mn _{1/4} Nb _{1/2} O ₃ Pb	CH ₃ NH ₃ Al(SO ₄) ₂ · 12H ₂ O	18A-4	158
157	Mg _{1/4} Mn _{1/4} O ₃ PbTa _{1/2}	Pb(Mg _{1/4} Mn _{1/4} Nb _{1/2})O ₃	1B3-xvii	70
157	Mg _{1/4} Mn _{1/4} O ₃ PbW _{1/2}	Pb(Mg _{1/4} Mn _{1/4} Ta _{1/2})O ₃	1B3-xvii	70
104	Mg _{1/4} Nb _{2/3} O ₃ Pb	Pb(Mg _{1/4} Mn _{1/4} W _{1/2})O ₃	1B3-xvii	70
104	MgNb ₁₄ O ₄₅ Sr ₉	Pb(Mg _{1/3} Nb _{2/3})O ₃	1B4-i	70
67	Mg _{1/3} O ₃ PbTa _{2/3}	Sr ₉ MgNb ₁₄ O ₄₅	5C-e2	104
104	Mg _{1/2} O ₃ PbW _{1/2}	Pb(Mg _{1/3} Ta _{2/3})O ₃	1B4-vi	72
104	Mn _{1/4} Nb _{1/2} Ni _{1/4} O ₃ Pb	Pb(Mg _{1/2} W _{1/2})O ₃	1B2-i	65
69	Mn _{1/2} Nb _{1/2} O ₃ Pb	Pb(Ni _{1/4} Mn _{1/4} Nb _{1/2})O ₃	1B3-xvii	70
70	Mn _{1/4} Nb _{1/2} O ₃ PbZn _{1/4}	Pb(Mn _{1/2} Nb _{1/2})O ₃	1B3-ii	67
73	Mn _{1/4} Ni _{1/4} O ₂ PbW _{1/2}	Pb(Zn _{1/4} Mn _{1/4} Nb _{1/2})O ₃	1B3-xvii	70
		Pb(Ni _{1/4} Mn _{1/4} W _{1/2})O ₃	1B3-xvii	70

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Gross formula	Chemical formula	Nr.	Page
MnO ₂	MnO ₂	35-31	212
Mn _{1/2} O ₃ PbRe _{1/2}	Pb(Mn _{1/2} Re _{1/2})O ₃	1B2-v	66
Mn _{1/2} O ₃ PbTa _{1/2}	Pb(Mn _{1/2} Ta _{1/2})O ₃	1B3-xi	69
Mn _{1/2} O ₃ PbW _{1/2}	Pb(Mn _{1/2} W _{1/2})O ₃	1B2-iii	66
Mn _{2/3} O ₃ PbW _{1/3}	Pb(Mn _{2/3} W _{1/3})O ₃	1B5-i	73
MnO ₃ Tm	TmMnO ₃	4A-4	96
MnO ₃ Y	YMnO ₃	4A-1	94
MnO ₃ Yb	YbMnO ₃	4A-5	96
Mo ₃ O ₁₂ Sm ₂	Sm ₂ (MoO ₄) ₃	35-1	200
Mo ₃ O ₁₂ Tb ₂	Tb ₂ (MoO ₄) ₃	35-4	201
NNaO ₂	NaNO ₂	11A-1	128
NO ₃ Rb	RbNO ₃	12A-2	133
NaNbO ₃	NaNbO ₃	1A-1	37
NaO ₃ Ta	NaTaO ₃	1A-3	40
NaO ₃ V	NaVO ₃	35-19	208
Nb _{1/2} Ni _{1/2} O ₃ Pb	Pb(Ni _{1/2} Nb _{1/2})O ₃	1B3-v	68
Nb _{2/3} Ni _{1/3} O ₃ Pb	Pb(Ni _{1/3} Nb _{2/3})O ₃	1B4-v	72
Nb ₂ O ₆ Pb	PbNb ₂ O ₆	5A-1	97
Nb ₂ O ₆ Pb ₂	Pb ₂ Nb ₂ O ₇	6A-2	106
Nb _{1/2} O ₃ PbSc _{1/2}	Pb(Sc _{1/2} Nb _{1/2})O ₃	1B3-i	67
Nb _{1/2} O ₃ PbYb _{1/2}	Pb(Yb _{1/2} Nb _{1/2})O ₃	1B3-vii	68
Nb _{2/3} O ₃ PbZn _{1/3}	Pb(Zn _{1/3} Nb _{2/3})O ₃	1B4-ii	71
Nb ₅ O ₁₅ RbSr ₂	RbSr ₂ Nb ₅ O ₁₅	5C-b4	103
Ni _{1/3} O ₃ PbTa _{2/3}	Pb(Ni _{1/3} Ta _{2/3})O ₃	1B4-viii	73
O ₃ PbSc _{1/2} Ta _{1/2}	Pb(Sc _{1/2} Ta _{1/2})O ₃	1B3-x	69
O ₆ Pb ₄ Si	Pb ₄ SiO ₆	35-26	210
O ₆ PbTa ₂	PbTa ₂ O ₆	5A-4	98
O ₃ PbTa _{1/2} Yb _{1/2}	Pb(Yb _{1/2} Ta _{1/2})O ₃	1B3-xiv	70
O ₃ PbTi	PbTiO ₃	1A-9	59
O ₈ Pb ₃ V ₂	Pb ₃ V ₂ O ₈	35-25	210
O ₃ PbZr	PbZrO ₃	1A-13	61
O ₃ RbTa	RbTaO ₃	35-17	207
O ₂ Sn	SnO ₂	35-32	212
O ₆ SrTa ₂	SrTa ₂ O ₆	5A-2	98
O ₇ Sr ₂ Ta ₂	Sr ₂ Ta ₂ O ₇	6A-3	106
O ₃ SrTi	SrTiO ₃	1A-6	45
O ₃ SrZr	SrZrO ₃	1A-11	61
O ₂ Ti	TiO ₂	35-30	212
O ₃ W	WO ₃	2A-1	88
p-azoxyanisole	C ₁₄ H ₁₄ N ₂ O ₃	37-1	215
p-azoxyphenetole	C ₁₆ H ₁₈ N ₂ O ₃	37-2	215
p-butoxybenzoic acid	C ₁₁ H ₁₄ O ₃	37-3	215
Perovskite	CaTiO ₃	1A-5	44
p-methoxycinnamic acid	C ₁₀ H ₁₀ O ₃	37-4	216
Pyrolusite	MnO ₂	35-31	212
Rochelle salt	NaKC ₄ H ₄ O ₆ · 4H ₂ O	33A-1	193
RS	NaKC ₄ H ₄ O ₆ · 4H ₂ O	33A-1	193
Rutile	TiO ₂	35-30	212
Seignette salt	NaKC ₄ H ₄ O ₆ · 4H ₂ O	33A-1	193
SiV ₃	V ₃ Si	36-4	214
SnTe	SnTe	36-2	213
TGS	(NH ₂ CH ₂ COOH) ₃ H ₂ SO ₄	28A-1	185
Tri-glycine tellurate		28A-4	190

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VB Solid solutions

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ABO_3	$\text{ABO}_3\text{-PbTiO}_3\text{-PbZrO}_3$	1C-f9	87
Al_2BaO_4	$\text{BaAl}_2\text{O}_4\text{-BaLi}_2\text{F}_4$	8B-1	115
AlLaO_3	$\text{LaAlO}_3\text{-BaTiO}_3$	1C-c8	83
AlLaO_3	$\text{LaAlO}_3\text{-BiFeO}_3$	1C-b11	83
AlLaO_3	$\text{LaAlO}_3\text{-PbTiO}_3$	1C-c10	84
AsH_6NO_4	$\text{NH}_4\text{H}_2\text{AsO}_4\text{-TlH}_2\text{AsO}_4$	13B-3	148
$\text{AsH}_2\text{O}_4\text{Tl}$	$\text{TlH}_2\text{AsO}_4\text{-NH}_4\text{H}_2\text{AsO}_4$	13B-3	148
AsIS	AsSI-SbSI	10B-1	127
$\text{BaBi}_2\text{Nb}_2\text{O}_9$	$(\text{Ba-Pb})\text{Bi}_2\text{Nb}_2\text{O}_9$	7B-5	114
$\text{BaBi}_2\text{Nb}_2\text{O}_9$	$\text{Bi}_2\text{BaNb}_2\text{O}_9\text{-Bi}_3\text{TiNbO}_9$	7B-1	113
$\text{BaBi}_3\text{NbO}_{12}\text{Ti}_2$	$\text{Bi}_3\text{BaTi}_2\text{NbO}_{12}\text{-Bi}_4\text{Ti}_3\text{O}_{12}$	7B-2	113
BaF_4Li_2	$\text{BaLi}_2\text{F}_4\text{-BaAl}_2\text{O}_4$	8B-1	115
$\text{BaFe}_{1/2}\text{O}_3\text{Ta}_{1/2}$	$\text{Ba}(\text{Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3\text{-BaTiO}_3$	1C-d2	84
BaHfO_3	$\text{BaHfO}_3\text{-BaTiO}_3$	1C-a24	77
BaHfO_3	$\text{BaHfO}_3\text{-PbHfO}_3$	1C-a18	76
BaNb_2O_6	$\text{BaNb}_2\text{O}_6\text{-BaTiO}_3$	1C-e9	86
BaNb_2O_6	$\text{BaNb}_2\text{O}_6\text{-BaZrO}_3$	5C-j2	105
BaNb_2O_6	$\text{BaNb}_2\text{O}_6\text{-CaNb}_2\text{O}_6$	5B-1	99
BaNb_2O_6	$\text{BaNb}_2\text{O}_6\text{-PbNb}_2\text{O}_6$	5B-5	100
BaNb_2O_6	$\text{BaNb}_2\text{O}_6\text{-SrNb}_2\text{O}_6$	5B-3	99
BaNb_2O_6	$\text{BaNb}_2\text{O}_6\text{-BaTiO}_3\text{-PbTiO}_3\text{-PbNb}_2\text{O}_6$	1C-f19	88
BaNb_2O_6	$(\text{Ba-Pb-Sr})(\text{Nb-Ta})_2\text{O}_6$	5B-15	102
BaNb_2O_6	$(\text{Ba-Pb-Ca})(\text{Nb-Ta})_2\text{O}_6$	5B-15	102
BaO_3Sn	$\text{BaZr}_{0.25}\text{Nb}_{1.5}\text{O}_{5.25}$	5C-j3	105
BaO_3Sn	$\text{BaSnO}_3\text{-BaTiO}_3$	1C-a25	77
BaO_3Sn	$\text{BaSnO}_3\text{-PbO:SnO}_2$	1C-a21	76
BaO_3Sn	$\text{BaSnO}_3\text{-PbTiO}_3$	1C-b10	83
BaO_3Sn	$(\text{Ba-Pb})(\text{Sn-Ti})\text{O}_3$	1C-f18	88
BaO_3Sn	$\text{BaSnO}_3\text{-SrSnO}_3$	1C-a20	76
BaO_6Ta_2	$\text{BaSnO}_3\text{-CaSnO}_3\text{-SrSnO}_3$	1C-f13	88
BaO_6Ta_2	$\text{BaTa}_2\text{O}_6\text{-BaTiO}_3$	1C-e10	87
BaO_6Ta_2	$(\text{Ba-Pb-Ca})(\text{Ta-Nb})_2\text{O}_6$	5B-15	102
BaO_6Ta_2	$(\text{Ba-Pb-Sr})(\text{Ta-Nb})_2\text{O}_6$	5B-15	102
BaO_3Ti	$\text{BaTiO}_3\text{-Ba}(\text{Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$	1C-d2	84
BaO_3Ti	$\text{BaTiO}_3\text{-BaHfO}_3$	1C-a24	77
BaO_3Ti	$\text{BaTiO}_3\text{-BaNb}_2\text{O}_6$	1C-e9	86
BaO_3Ti	$\text{BaTiO}_3\text{-BaSnO}_3$	1C-a25	77
BaO_3Ti	$\text{BaTiO}_3\text{-BaTa}_2\text{O}_6$	1C-e10	87
BaO_3Ti	$\text{BaTiO}_3\text{-BaUO}_3$	1C-a26	77
BaO_3Ti	$\text{BaTiO}_3\text{-BaZrO}_3$	1C-a23	77
BaO_3Ti	$\text{BaTiO}_3\text{-BiFeO}_3$	1C-c9	84
BaO_3Ti	$\text{BaTiO}_3\text{-Bi}_4\text{Ti}_3\text{O}_{12}$	7B-6	114
BaO_3Ti	$\text{BaTiO}_3\text{-CaTiO}_3$	1C-a7	74
BaO_3Ti	$\text{BaTiO}_3\text{-Co}_2\text{Nb}_2\text{O}_7$	1C-e11	87
BaO_3Ti	$\text{BaTiO}_3\text{-Co}_2\text{Ta}_2\text{O}_7$	1C-e11	87
BaO_3Ti	$\text{BaTiO}_3\text{-(K}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$	1C-e11	87
BaO_3Ti	$\text{BaTiO}_3\text{-KNbO}_3$	1C-d3	84
BaO_3Ti	$\text{BaTiO}_3\text{-LaAlO}_3$	1C-c5	83
BaO_3Ti	$\text{BaTiO}_3\text{-Mn}_2\text{Nb}_2\text{O}_7$	1C-c8	83
BaO_3Ti	$\text{BaTiO}_3\text{-Mn}_2\text{Ta}_2\text{O}_7$	1C-e11	87
BaO_3Ti	$\text{BaTiO}_3\text{-NaNbO}_3$	1C-e11	87
BaO_3Ti	$\text{BaTiO}_3\text{-Ni}_2\text{Nb}_2\text{O}_7$	1C-c2	83
BaO_3Ti	$\text{BaTiO}_3\text{-Ni}_2\text{Ta}_2\text{O}_7$	1C-e11	87
BaO_3Ti	$\text{BaTiO}_3\text{-PbO:SnO}_2$	1C-b4	82
BaO_3Ti	$\text{BaTiO}_3\text{-PbTiO}_3$	1C-a11	75
BaO_3Ti	$\text{BaTiO}_3\text{-PbZrO}_3$	1C-b3	82
BaO_3Ti	$\text{BaTiO}_3\text{-SrTiO}_3$	1C-a9	75
BaO_3Ti	$\text{BaTiO}_3\text{-CaTiO}_3\text{-PbTiO}_3$	1C-f2	87
BaO_3Ti	$\text{BaTiO}_3\text{-CaTiO}_3\text{-SrTiO}_3$	1C-f1	87

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Gross formula	Chemical formula	Nr.	Page
BaO ₃ Ti	BaTiO ₃ -LaInO ₃ -LaYO ₃ -SrTiO ₃	1C-f12	88
BaO ₃ Ti	BaTiO ₃ -PbTiO ₃ -BaNb ₂ O ₆ -PbNb ₂ O ₆	1C-f19	88
BaO ₃ Ti	(Ba-Ca)(Ti-Zr)O ₃	1C-f15	88
BaO ₃ Ti	(Ba-Pb)(Ti-Sn)O ₃	1C-f18	88
BaO ₃ Ti	(Ba-Pb)(Ti-Zr)O ₃	1C-f17	88
BaO ₃ U	BaUO ₃ -BaTiO ₃	1C-a26	77
BaO ₃ Zr	BaZrO ₃ -BaNb ₂ O ₆	5C-j2	105
BaO ₃ Zr	BaZrO ₃ -BaTiO ₃	1C-a23	77
BaO ₃ Zr	BaZrO ₃ -CaZrO ₃	1C-a12	76
BaO ₃ Zr	BaZrO ₃ -PbTiO ₃	1C-b9	82
BaO ₃ Zr	BaZrO ₃ -PbZrO ₃	1C-a15	76
BaO ₃ Zr	(Ba-Ca)(Zr-Ti)O ₃	1C-f15	88
BaO ₃ Zr	(Ba-Pb)(Zr-Ti)O ₃	1C-f17	88
BaO ₃ Zr	BaZr _{0.25} Nb _{1.5} O _{5.25}	5C-j3	105
BeF ₄ H ₈ N ₂	(NH ₄) ₂ BeF ₄ -(NH ₄) ₂ SO ₄	14B-1	154
BiFeO ₃	BiFeO ₃ -BaTiO ₃	1C-c9	84
BiFeO ₃	BiFeO ₃ -LaAlO ₃	1C-b11	83
BiFeO ₃	BiFeO ₃ -LaCrO ₃	1C-b12	83
BiFeO ₃	BiFeO ₃ -LaFeO ₃	1C-a33	82
BiFeO ₃	BiFeO ₃ -Pb(Fe _{1/2} Nb _{1/2})O ₃	1C-d23	85
BiFeO ₃	BiFeO ₃ -PbTiO ₃	1C-c13	84
BiFeO ₃	BiFeO ₃ -PbZrO ₃	1C-c14	84
BiFeO ₃	BiFeO ₃ -SrFeO ₃	1C-c16	84
BiFeO ₃	BiFeO ₃ -Sr(Sn _{1/3} Mn _{2/3})O ₃	1C-d22	85
BiFeO ₃	BiFeO ₃ -SrSnO ₃	1C-c15	84
BiFeO ₃	BiFeO ₃ -SrTiO ₃	1C-c7	83
BiFeO ₃	BiFeO ₃ -PbTiO ₃ -PbZrO ₃	1C-f6	87
Bi ₅ GaO ₁₅ Ti ₃	Bi ₅ Ti ₃ GaO ₁₅ -Bi ₄ PbTi ₄ O ₁₅	7B-7	114
BiSI	BiSI-SbSI	10B-5	128
Bi _{1/2} K _{1/2} O ₃ Ti	(K _{1/2} Bi _{1/2})TiO ₃ -BaTiO ₃	1C-d3	84
Bi _{1/2} K _{1/2} O ₃ Ti	(K _{1/2} Bi _{1/2})TiO ₃ -(Na _{1/2} Bi _{1/2})TiO ₃	1C-d20	85
Bi _{1/2} K _{1/2} O ₃ Ti	(K _{1/2} Bi _{1/2})TiO ₃ -PbTiO ₃	1C-d5	84
Bi _{1/2} K _{1/2} O ₃ Zr	(K _{1/2} Bi _{1/2})ZrO ₃ -PbZrO ₃	1C-d17	85
Bi _{1/2} Na _{1/2} O ₃ Ti	(Na _{1/2} Bi _{1/2})TiO ₃ -(K _{1/2} Bi _{1/2})TiO ₃	1C-d20	85
Bi _{1/2} Na _{1/2} O ₃ Ti	(Na _{1/2} Bi _{1/2})TiO ₃ -PbTiO ₃	1C-d4	84
Bi _{1/2} Na _{1/2} O ₃ Ti	(Na _{1/2} Bi _{1/2})TiO ₃ -PbZrO ₃	1C-d21	85
Bi _{1/2} Na _{1/2} O ₃ Zr	(Na _{1/2} Bi _{1/2})ZrO ₃ -PbZrO ₃	1C-d16	85
BiNbO ₆	Bi(Nb-Ti)O ₆ -PbNb ₂ O ₆	5B-14	102
Bi ₂ Nb ₆ O ₁₈	Bi ₂ O ₉ · 3Nb ₂ O ₅ -PbNb ₂ O ₆	5B-13	102
Bi ₂ Nb ₂ O ₉ Pb	Bi ₂ PbNb ₂ O ₉ -Bi ₃ TiNbO ₉	7B-1	113
Bi ₂ Nb ₂ O ₉ Pb	Bi ₂ PbNb ₂ O ₉ -BaBi ₂ Nb ₂ O ₉	7B-5	114
Bi ₃ NbO ₁₂ PbTi ₂	Bi ₃ PbTi ₂ NbO ₁₂ -Bi ₄ Ti ₃ O ₁₂	7B-2	113
Bi ₂ Nb ₂ O ₉ Sr	Bi ₂ SrNb ₂ O ₉ -Bi ₃ TiNbO ₉	7B-1	113
Bi ₃ NbO ₁₂ SrTi ₂	Bi ₃ SrTi ₂ NbO ₁₂ -Bi ₄ Ti ₃ O ₁₂	7B-2	113
Bi ₃ NbO ₉ Ti	Bi ₃ TiNbO ₉ -Bi ₂ BaNb ₂ O ₉	7B-1	113
Bi ₃ NbO ₉ Ti	Bi ₃ TiNbO ₉ -Bi ₂ PbNb ₂ O ₉	7B-1	113
Bi ₃ NbO ₉ Ti	Bi ₃ TiNbO ₉ -Bi ₂ SrNb ₂ O ₉	7B-1	113
Bi ₄ O ₁₅ PbTi ₄	Bi ₄ PbTi ₄ O ₁₅ -Bi ₅ Ti ₃ GaO ₁₅	7B-7	114
BiO ₂ Ti	Bi(Ti-Nb)O ₆ -PbNb ₂ O ₆	5B-14	102
Bi ₂ O ₉ Ti ₃	Bi ₂ O ₉ · 3TiO ₂ -PbNb ₂ O ₆	5B-14	102
Bi ₂ O ₉ Ti ₃	Bi ₂ O ₉ · 3TiO ₂ -SrTiO ₃	1C-e8	86
Bi ₄ O ₁₂ Ti ₃	Bi ₄ Ti ₃ O ₁₂ -BaTiO ₃	7B-6	114
Bi ₄ O ₁₂ Ti ₃	Bi ₄ Ti ₃ O ₁₂ -Bi ₃ BaTi ₂ NbO ₁₂	7B-2	113
Bi ₄ O ₁₂ Ti ₃	Bi ₄ Ti ₃ O ₁₂ -Bi ₃ PbTi ₂ NbO ₁₂	7B-2	113
Bi ₄ O ₁₂ Ti ₃	Bi ₄ Ti ₃ O ₁₂ -Bi ₃ SrTi ₂ NbO ₁₂	7B-2	113
BrSSb	SbSBr-SbSI	10B-3	127
C ₆ FH ₁₇ N ₃ O ₉ P	(NH ₄ CH ₂ COOH) ₅ · H ₂ PO ₄ F-	28B-2	191
C ₆ FeH ₆ K ₄ N ₆ O ₃	(NH ₄ CH ₂ COOH) ₅ · H ₂ SO ₄	22B-1	176
C ₆ FeH ₆ K ₄ N ₆ O ₃	K ₄ Fe(CN) ₆ · 3H ₂ O-(NH ₄) ₄ Fe(CN) ₆ · 3H ₂ O	22B-2	176
C ₆ FeH ₆ K ₄ N ₆ O ₃	K ₄ Fe(CN) ₆ · 3H ₂ O-Rb ₄ Fe(CN) ₆ · 3H ₂ O	22B-3	177
C ₆ FeH ₁₆ N ₁₀ · 3H ₂ O	K ₄ Fe(CN) ₆ · 3H ₂ O-Tl ₄ Fe(CN) ₆ · 3H ₂ O	22B-1	176
C ₆ FeH ₂₂ N ₁₀ O ₃	(NH ₄) ₄ Fe(CN) ₆ · 3H ₂ O-K ₄ Fe(CN) ₆ · 3H ₂ O	22B-1	176

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$C_6FeH_6N_6O_4Rb_4$	$Rb_4Fe(CN)_6 \cdot 3H_2O - K_4Fe(CN)_6 \cdot 3H_2O$	22B-2	176
$C_6FeH_6N_6O_3Tl_4$	$Tl_4Fe(CN)_6 \cdot 3H_2O - K_4Fe(CN)_6 \cdot 3H_2O$	22B-3	177
$C_6FeK_4N_6 \cdot 3H_2O$	$K_4Fe(CN)_6 \cdot 3H_2O - (NH_4)_4Fe(CN)_6 \cdot 3H_2O$	22B-1	176
$C_6FeK_4N_6 \cdot 3H_2O$	$K_4Fe(CN)_6 \cdot 3H_2O - Rb_4Fe(CN)_6 \cdot 3H_2O$	22B-2	176
$C_6FeK_4N_6 \cdot 3H_2O$	$K_4Fe(CN)_6 \cdot 3H_2O - Tl_4Fe(CN)_6 \cdot 3H_2O$	22B-3	177
$C_6FeN_6Rb_4 \cdot 3H_2O$	$Rb_4Fe(CN)_6 \cdot 3H_2O - K_4Fe(CN)_6 \cdot 3H_2O$	22B-2	176
$C_6FeN_6Tl_4 \cdot 3H_2O$	$Tl_4Fe(CN)_6 \cdot 3H_2O - K_4Fe(CN)_6 \cdot 3H_2O$	22B-3	177
$C_6H_4KNaO_6 \cdot 4H_2O$	$NaKC_4H_4O_6 \cdot 4H_2O - NaNH_4C_4H_4O_6 \cdot 4H_2O$	33B-1	198
$C_6H_4KNaO_6 \cdot 4H_2O$	$NaKC_4H_4O_6 \cdot 4H_2O - NaTiC_4H_4O_6 \cdot 4H_2O$	33B-2	198
$C_6H_{12}KNaO_{10}$	$NaKC_4H_4O_6 \cdot 4H_2O - NaNH_4C_4H_4O_6 \cdot 4H_2O$	33B-1	198
$C_6H_{12}KNaO_{10}$	$NaKC_4H_4O_6 \cdot 4H_2O - NaTiC_4H_4O_6 \cdot 4H_2O$	33B-2	198
$C_6H_8NNaO_6 \cdot 4H_2O$	$NaNH_4C_4H_4O_6 \cdot 4H_2O - NaKC_4H_4O_6 \cdot 4H_2O$	33B-1	198
$C_6H_{16}NNaO_{10}$	$NaNH_4C_4H_4O_6 \cdot 4H_2O - NaKC_4H_4O_6 \cdot 4H_2O$	33B-1	198
$C_6H_{17}N_3O_{10}S$	$(NH_2CH_2COOH)_3 \cdot H_2SO_4 - (NH_2CH_2COOH)_3 \cdot H_2PO_3F$	28B-2	191
$C_6H_{17}N_3O_{10}S$	$(NH_2CH_2COOH)_3 \cdot H_2SeO_4 - (NH_2CH_2COOH)_3 \cdot H_2SeO_4$	28B-1	191
$C_6H_{17}N_3O_{10}Se$	$(NH_2CH_2COOH)_3 \cdot H_2SeO_4 - (NH_2CH_2COOH)_3 \cdot H_2SO_4$	28B-1	191
$C_6H_4NaO_6Tl \cdot 4H_2O$	$NaTiC_4H_4O_6 \cdot 4H_2O - NaKC_4H_4O_6 \cdot 4H_2O$	33B-2	198
$C_6H_{12}NaO_{10}Tl$	$NaTiC_4H_4O_6 \cdot 4H_2O - NaKC_4H_4O_6 \cdot 4H_2O$	33B-2	198
$CaHfO_3$	$CaHfO_3 - PbHfO_3$	1C-a16	76
$CaNb_2O_6$	$CaNb_2O_6 - BaNb_2O_6$	5B-1	99
$CaNb_2O_6$	$CaNb_2O_6 - NaNbO_3$	1C-e3	86
$CaNb_2O_6$	$CaNb_2O_6 - PbNb_2O_6$	5B-2	99
$CaNb_2O_6$	$(Ca - Ba - Pb)(Nb - Ta)_2O_6$	5B-15	102
$Ca_2Nb_2O_7$	$Ca_2Nb_2O_7 - Cd_2Nb_2O_7$	6B-1	106
CaO_3Sn	$CaSnO_3 - PbTiO_3$	1C-b6	82
CaO_3Sn	$CaSnO_3 - SrSnO_3$	1C-a19	76
CaO_3Sn	$CaSnO_3 - SrSnO_3 - BaSnO_3$	1C-f13	88
CaO_6Ta_2	$(Ca - Ba - Pb)(Ta - Nb)_2O_6$	5B-15	102
$Ca_2O_7Ta_2$	$Ca_2Ta_2O_7 - Sr_2Ta_2O_7$	6B-6	106
CaO_3Ti	$CaTiO_3 - BaTiO_3$	1C-a7	74
CaO_3Ti	$CaTiO_3 - CaZrO_3$	1C-a22	76
CaO_3Ti	$CaTiO_3 - NaNbO_3$	1C-c1	83
CaO_3Ti	$CaTiO_3 - PbTiO_3$	1C-a8	75
CaO_3Ti	$CaTiO_3 - SrTiO_3$	1C-a6	74
CaO_3Ti	$CaTiO_3 - BaTiO_3 - PbTiO_3$	1C-f2	87
CaO_3Ti	$CaTiO_3 - BaTiO_3 - SrTiO_3$	1C-f1	87
CaO_3Ti	$(Ca - Ba)(Ti - Zr)O_3$	1C-f15	88
CaO_3Zr	$CaZrO_3 - BaZrO_3$	1C-a12	76
CaO_3Zr	$CaZrO_3 - CaTiO_3$	1C-a22	76
CaO_3Zr	$CaZrO_3 - PbTiO_3$	1C-b5	82
CaO_3Zr	$CaZrO_3 - PbZrO_3$	1C-a13	76
CaO_3Zr	$(Ca - Ba)(Zr - Ti)O_3$	1C-f15	88
$CdNb_2O_6$	$CdNb_2O_6 - NaNbO_3$	1C-e4	86
$CdNb_2O_6$	$CdNb_2O_6 - PbNb_2O_6$	5B-10	101
$Cd_2Nb_2O_7$	$Cd_2Nb_2O_7 - Ca_2Nb_2O_7$	6B-1	106
$Cd_2Nb_2O_7$	$Cd_2Nb_2O_7 - Cd_2Ta_2O_7$	6B-3	106
$Cd_2Nb_2O_7$	$Cd_4Nb_2O_7 - Mg_2Nb_2O_7$	6B-4	106
$Cd_2Nb_2O_7$	$Cd_2Nb_2O_7 - Pb_2Nb_2O_7$	6B-2	106
$Cd_2O_3Ta_2$	$Cd_2Ta_2O_7 - Cd_2Nb_2O_7$	6B-3	106
CdO_3Ti	$CdTiO_3 - LiNbO_3$	1C-e7	86
CdO_3Ti	$CdTiO_3 - LiTaO_3$	1C-e7	86
$Ce_{1/2}Li_{1/2}O_3Ti$	$(Li_{1/2}Ce_{1/2})TiO_5 - PbTiO_3$	1C-d8	85
$CoLaO_3$	$LaCoO_3 - PbTiO_3 - LaMnO_3$	1C-f11	87
$Co_2Nb_2O_7$	$Co_2Nb_2O_7 - BaTiO_3$	1C-e11	87
$Co_2O_3Ta_2$	$Co_2Ta_2O_7 - BaTiO_3$	1C-e11	87
$CrLaO_3$	$LaCrO_3 - BiFeO_3$	1C-b12	83
$CrLaO_3$	$LaCrO_3 - PbTiO_3 - LaMnO_3$	1C-f11	87
$CsNO_3$	$CsNO_3 - RbNO_3$	12B-4	134
$Eu_2Mo_3O_{12}$	$(Eu - Gd)_2(MoO_4)_3$	35-5	201
$Eu_2Mo_3O_{12}$	$(Eu - Tb)_2(MoO_4)_3$	35-6	201

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Gross formula	Chemical formula	Nr.	Page
FeLaO ₃	LaFeO ₃ -BiFeO ₃	1C-a33	82
FeLaO ₃	LaFeO ₃ -PbTiO ₃	1C-c12	84
FeLaO ₃	LaFeO ₃ -PbTiO ₃ -LaMnO ₃	1C-f11	87
FeLaO ₃	LaFeO ₃ -PbTiO ₃ -PbZrO ₃	1C-f5	87
Fe _{1/2} Nb _{1/2} O ₃ Pb	Pb(Fe _{1/2} Nb _{1/2})O ₃ -BiFeO ₃	1C-d23	85
Fe _{1/2} Nb _{1/2} O ₃ Pb	Pb(Fe _{1/2} Nb _{1/2})O ₃ -PbTiO ₃ -PbZrO ₃	1C-f8	87
Fe _{1/2} O ₃ PbTa _{1/2}	Pb(Fe _{1/2} Ta _{1/2})O ₃ -PbTiO ₃	1C-d11	85
Fe _{1/2} O ₃ PbTa _{1/2}	Pb(Fe _{1/2} Ta _{1/2})O ₃ -PbZrO ₃	1C-d15	85
FeO ₃ Sr	SrFeO ₃ -BiFeO ₃	1C-c16	84
Fe _{1/2} O ₃ SrTa _{1/2}	Sr(Fe _{1/2} Ta _{1/2})O ₃ -SrTiO ₃	1C-d1	84
Gd ₂ Mo ₃ O ₁₂	(Gd-Eu) ₂ (MoO ₄) ₃	35-5	201
Gd ₂ Mo ₃ O ₁₂	(Gd-Nd) ₂ (MoO ₄) ₃	35-8	202
Gd ₂ Mo ₃ O ₁₂	(Gd-Tb) ₂ (MoO ₄) ₃	35-9	202
Gd ₂ Mo ₃ O ₁₂	(Gd-Y) ₂ (MoO ₄) ₃	35-7	202
Gd ₂ Mo ₃ O ₁₂	Gd ₂ ((Mo-W)O ₄) ₃	35-10	202
Gd ₂ O ₁₂ W ₃	Gd ₂ ((W-Mo)O ₄) ₃	35-10	202
GeTe	GeTe-SnTe	36-3	214
H ₂ KO ₄ P	KH ₂ PO ₄ -NH ₄ H ₂ PO ₄	13B-1	148
H ₄ N ₂ O ₃	NH ₄ NO ₃ -KNO ₃	12B-1	134
H ₆ NO ₄ P	NH ₄ H ₂ PO ₄ -KH ₂ PO ₄	13B-1	148
H ₆ NO ₄ P	NH ₄ H ₂ PO ₄ -TiH ₂ PO ₄	13B-2	148
H ₈ N ₂ O ₄ S	(NH ₄) ₂ SO ₄ -(NH ₄) ₂ BeF ₄	14B-1	154
H ₂ O ₄ PTl	TlH ₂ PO ₄ -NH ₄ H ₂ PO ₄	13B-2	148
HfO ₃ Pb	PbHfO ₃ -BaHfO ₃	1C-a18	76
HfO ₃ Pb	PbHfO ₃ -CaHfO ₃	1C-a16	76
HfO ₃ Pb	PbHfO ₃ -Pb(Sc _{1/2} Nb _{1/2})O ₃	1C-d18	85
HfO ₃ Pb	PbHfO ₃ -PbTiO ₃	1C-a29	82
HfO ₃ Pb	PbHfO ₃ -PbZrO ₃	1C-a31	82
HfO ₃ Pb	PbHfO ₃ -SrHfO ₃	1C-a17	76
HfO ₃ Pb	PbHfO ₃ -PbTiO ₃ -PbO:SnO ₂	1C-f4	87
HfO ₃ Sr	SrHfO ₃ -PbHfO ₃	1C-a17	76
IK	KI-KNO ₃	12B-3	134
IOSb	SbOI-SbSI	10B-2	127
ISSb	SbSI-AsSI	10B-1	127
ISSb	SbSI-BiSI	10B-5	128
ISSb	SbSI-SbOI	10B-2	127
ISSb	SbSI-SbSBr	10B-3	127
ISSb	SbSI-SbSeI	10B-4	128
ISbSe	SbSeI-SbSI	10B-4	128
InLaO ₃	LaInO ₃ -BaTiO ₃ -LaYO ₃ -SrTiO ₃	1C-f12	88
KNO ₃	KNO ₃ -KI	12B-3	134
KNO ₃	KNO ₃ -NH ₄ NO ₃	12B-1	134
KNO ₃	KNO ₃ -RbNO ₃	12B-2	134
KNbO ₃	KNbO ₃ -BaTiO ₃	1C-c5	83
KNbO ₃	KNbO ₃ -KTaO ₃	1C-a4	74
KNbO ₃	KNbO ₃ -NaNbO ₃	1C-a1	73
KNbO ₃	KNbO ₃ -PbNb ₂ O ₆	5B-11	101
KNbO ₃	KNbO ₃ -PbTiO ₃	1C-c6	83
KNbO ₃	KNbO ₃ -SrNb ₂ O ₆	5C-b6	103
KNbO ₃	(K-Na)(Nb-Ta)O ₃	1C-f14	88
KNbO ₃	K _{0.6} Li _{0.4} (Nb _{0.3} Ta _{0.7})O ₃	5C-k2	105
KNbO ₃	K(Nb _{0.65} Ta _{0.35})O ₃ (KTN)	1C-a5	74
KO ₃ Sb	KSbO ₃ -NaNbO ₃	1C-b2	82
KO ₃ Ta	KTaO ₃ -KNbO ₃	1C-a4	74
KO ₃ Ta	KTaO ₃ -NaNbO ₃	1C-b1	82
KO ₃ Ta	K(Ta _{0.35} Nb _{0.65})O ₃ (KTN)	1C-a5	74
KO ₃ Ta	(K-Na)(Ta _{0.7} Nb _{0.3})O ₃	1C-f14	88
KO ₃ Ta	K _{0.6} Li _{0.4} (Ta _{0.7} Nb _{0.3})O ₃	5C-k2	105
KTN	K(Ta _{0.35} Nb _{0.65})O ₃	1C-a5	74

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Page	Gross formula	Chemical formula	Nr.	Page
82	LaFeO ₃	LaFeO ₃ -PbTiO ₃	1C-c12	84
84	La _{1/2} Li _{1/2} O ₃ Ti	(Li _{1/2} La _{1/2})TiO ₃ -PbTiO ₃	1C-d6	84
87	LaMnO ₃	LaMnO ₃ -PbTiO ₃	1C-c11	84
87	LaMnO ₃	LaMnO ₃ -LaCoO ₃ -PbTiO ₃	1C-f11	87
85	LaMnO ₃	LaMnO ₃ -LaCrO ₃ -PbTiO ₃	1C-f11	87
87	LaMnO ₃	LaMnO ₃ -LaFeO ₃ -PbTiO ₃	1C-f11	87
85	LaMnO ₃	LaMnO ₃ -LaNiO ₃ -PbTiO ₃	1C-f11	87
85	LaMnO ₃	LaMnO ₃ -PbTiO ₃ -SrTiO ₃	1C-f10	87
84	La _{1/2} Na _{1/2} O ₃ Ti	(Na _{1/2} La _{1/2})TiO ₃ -PbTiO ₃	1C-d7	85
84	La ₂ Nb ₆ O ₁₈	La ₂ O ₃ ·3Nb ₂ O ₅ -PbNb ₂ O ₆	5B-12	101
201	LaNiO ₃	LaNiO ₃ -LaMnO ₃ -PbTiO ₃	1C-f11	87
202	LaO ₃ Y	LaYO ₃ -BaTiO ₃ -LaInO ₃ -SrTiO ₃	1C-f12	88
202	LiNbO ₃	LiNbO ₃ -CdTiO ₃	1C-e7	86
202	LiNbO ₃	LiNbO ₃ -LiTaO ₃	3B-1	94
202	LiNbO ₃	LiNbO ₃ -NaNbO ₃	1C-e1	86
202	LiNbO ₃	LiNbO ₃ -PbNb ₂ O ₆	5B-11	101
214	Li _{1/2} Nd _{1/2} O ₃ Ti	Li _{0.4} K _{0.6} (Nb _{0.3} Ta _{0.7})O ₃ (Li _{1/2} Nd _{1/2})TiO ₃ -PbTiO ₃	5C-k2	105
148	LiO ₃ Ta	LiTaO ₃ -CdTiO ₃	1C-d9	85
134	LiO ₃ Ta	LiTaO ₃ -LiNbO ₃	1C-e7	86
148	LiO ₃ Ta	Li _{0.4} K _{0.6} (Ta _{0.7} Nb _{0.3})O ₃	3B-1	94
148	Li _{0.4} K _{0.6} (Ta _{0.7} Nb _{0.3})O ₃	5C-k2	105	
148	Mg ₂ Nb ₂ O ₇	Mg ₂ Nb ₂ O ₇ -Cd ₂ Nb ₂ O ₆	6B-4	106
154	Mg _{1/3} Nb _{2/3} O ₃ Pb	Pb(Mg _{1/3} Nb _{2/3})O ₃ -Pb(Mg _{1/3} W _{1/2})O ₃	1C-d19	85
148	Mg _{1/3} Nb _{2/3} O ₃ Pb	Pb(Mg _{1/3} Nb _{2/3})O ₃ -PbTiO ₃ -PbZrO ₃	1C-f7	87
76	Mg _{1/2} O ₃ PbW _{1/2}	Pb(Mg _{1/2} W _{1/2})O ₃ -Pb(Mg _{1/3} Nb _{2/3})O ₃	1C-d19	85
76	Mg _{1/2} O ₃ PbW _{1/2}	Pb(Mg _{1/2} W _{1/2})O ₃ -PbTiO ₃	1C-d10	85
85	Mn _{1/2} Nb _{1/2} O ₃ Pb	Pb(Mn _{1/2} Nb _{1/2})O ₃ -PbTiO ₃	1C-d13	85
82	Mn _{2/3} O ₂ Sn _{1/3} Sr	Sr(Sn _{1/3} Mn _{2/3})O ₃ -BiFeO ₃	1C-d22	85
82	Mn ₂ Nb ₂ O ₇	Mn ₂ Nb ₂ O ₇ -BaTiO ₃	1C-e11	87
76	Mn ₂ O ₂ Ta ₂	Mn ₂ Ta ₂ O ₇ -BaTiO ₃	1C-e11	87
87	Mo ₃ Nd ₂ O ₁₂	(Nd-Gd) ₂ (MoO ₄) ₃	35-8	202
76	Mo ₃ O ₁₂ Tb ₂	(Tb-Eu) ₂ (MoO ₄) ₃	35-6	201
	Mo ₃ O ₁₂ Tb ₂	(Tb-Gd) ₂ (MoO ₄) ₃	35-9	202
	Mo ₃ O ₁₂ Y ₂	(Y-Gd) ₂ (MoO ₄) ₃	35-7	202
134	NO ₃ Rb	RbNO ₃ -CsNO ₃	12B-4	134
127	NO ₃ Rb	RbNO ₃ KNO ₃	12B-2	134
128	NaNbO ₃	NaNbO ₃ -BaTiO ₃	1C-c2	83
127	NaNbO ₃	NaNbO ₃ -CaNb ₂ O ₆	1C-e3	86
127	NaNbO ₃	NaNbO ₃ -CaTiO ₃	1C-c1	83
128	NaNbO ₃	NaNbO ₃ -CdNb ₂ O ₆	1C-e4	86
88	NaNbO ₃	NaNbO ₃ -KNbO ₃	1C-a1	73
134	NaNbO ₃	NaNbO ₃ -KSB ₃ O ₃	1C-b2	82
134	NaNbO ₃	NaNbO ₃ -KTaO ₃	1C-b1	82
134	NaNbO ₃	NaNbO ₃ -LiNbO ₃	1C-e1	86
83	NaNbO ₃	NaNbO ₃ -NaVO ₃	1C-e2	86
74	NaNbO ₃	NaNbO ₃ -NaSbO ₃	1C-a3	74
73	NaNbO ₃	NaNbO ₃ -NaTaO ₃	1C-a2	74
	NaNbO ₃	NaNbO ₃ -PbNb ₂ O ₆	1C-e6	86
101	NaNbO ₃	NaNbO ₃ -PbTiO ₃	5B-11	101
83	NaNbO ₃	NaNbO ₃ -PbZrO ₃	1C-c3	83
103	NaNbO ₃	NaNbO ₃ -SrNb ₂ O ₆	1C-c4	83
88	NaNbO ₃	(Na-K)(Nb-Ta)O ₃	1C-e5	86
105	NaO ₃ Sb	NaSbO ₃ -NaNbO ₃	1C-f14	88
74	NaO ₃ Ta	NaTaO ₃ -NaNbO ₃	1C-a3	74
82	NaO ₃ Ta	(Na-K)(Ta-Nb)O ₃	1C-a2	74
74	NaO ₃ V	NaVO ₃ -NaNbO ₃	1C-f14	88
82	Nb ₂ Ni ₂ O ₇	Ni ₂ Nb ₂ O ₇ -BaTiO ₃	1C-e2	86
74	Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -BaNb ₂ O ₆	1C-e11	87
88	Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -Bi ₂ O ₃ · 3Nb ₂ O ₆	5B-5	100
105	Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -Bi ₂ O ₃ · 3TiO ₂	5B-13	102
74	Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -CaNb ₂ O ₆	5B-14	102
	Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -CaNb ₂ O ₆	5B-2	99

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Gross formula	Chemical formula	Nr.	Page
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -CdNb ₂ O ₆	5B-10	101
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -KNbO ₃	5B-11	101
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -La ₂ O ₃ · 3Nb ₂ O ₅	5B-12	101
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -LiNbO ₃	5B-11	101
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -NaNbO ₃	1C-e6,	86
Nb ₂ O ₆ Pb		5B-11	101
Nb ₂ O ₆ Pb		5B-9	101
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -PbO : SnO ₂	5B-6	101
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -PbTa ₂ O ₆	5B-7	101
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -PbTiO ₃	5B-8,	101
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -PbZrO ₃	1C-e12	87
Nb ₂ O ₆ Pb		5B-11	101
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -RbNbO ₃	5B-12	101
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -Sm ₂ O ₃ · 3Nb ₂ O ₅	5B-4	100
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -SrNb ₂ O ₆	5B-12	101
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -Y ₂ O ₃ · 3Nb ₂ O ₅	5B-14	102
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -Bi(Nb-Ti)O ₆	1C-f19	88
Nb ₂ O ₆ Pb	PbNb ₂ O ₆ -BaNb ₂ O ₆ -BaTiO ₃ -PbTiO ₃	5B-15	102
Nb ₂ O ₆ Pb	(Pb-Ba-Ca)(Nb-Ta) ₂ O ₆	5B-15	102
Nb ₂ O ₆ Pb	(Pb-Ba-Sr)(Nb-Ta) ₂ O ₆	6B-2	106
Nb ₂ O ₆ Pb	Pb ₂ Nb ₂ O ₇ -Cd ₂ Nb ₂ O ₇	1C-d18	85
Nb ₂ O ₇ Pb ₂	Pb(Sc _{1/2} Nb _{1/2})O ₃ -PbHfO ₃	1C-d12	85
Nb _{1/2} O ₃ PbSc _{1/2}	Pb(Sc _{1/2} Nb _{1/2})O ₃ -PbTiO ₃	1C-d14	85
Nb _{1/2} O ₃ PbSc _{1/2}	Pb(Sc _{1/2} Nb _{1/2})O ₃ -PbZrO ₃	5B-11	101
Nb _{1/2} O ₃ PbSc _{1/2}	RbNbO ₃ -PbNb ₂ O ₆	5B-12	101
Nb ₄ O ₁₈ Sm ₂	Sm ₂ O ₃ · 3Nb ₂ O ₅ -PbNb ₂ O ₆	5B-3	99
Nb ₂ O ₆ Sr	SrNb ₂ O ₆ -BaNb ₂ O ₆	5C-b6	103
Nb ₂ O ₆ Sr	SrNb ₂ O ₆ -KNbO ₃	1C-e5	86
Nb ₂ O ₆ Sr	SrNb ₂ O ₆ -NaNbO ₃	5B-4	100
Nb ₂ O ₆ Sr	SrNb ₂ O ₆ -PbNb ₂ O ₆	5B-15	102
Nb ₂ O ₆ Sr	(Sr-Ba-Pb)(Nb-Ta) ₂ O ₆	6B-5	106
Nb ₂ O ₆ Sr	Sr ₂ Nb ₂ O ₇ -Sr ₂ Ta ₂ O ₇	1C-e11	87
Nb ₂ O ₇ Sr ₂	Sr ₂ Ta ₂ O ₇ -BaTiO ₃	5B-12	101
Ni ₂ O ₇ Ta ₂	Ni ₂ Ta ₂ O ₇ -BaTiO ₃	1C-a21	76
Nb ₂ O ₁₈ Y ₂	Y ₂ O ₃ · 3Nb ₂ O ₅ -PbNb ₂ O ₆	1C-b4	82
O ₃ PbSn	PbO : SnO ₂ -BaSnO ₃	5B-9	101
O ₃ PbSn	PbO : SnO ₂ -BaTiO ₃	1C-a30	82
O ₃ PbSn	PbO : SnO ₂ -PbNb ₂ O ₆	1C-a32	82
O ₃ PbSn	PbO : SnO ₂ -PbTiO ₃	1C-f4	87
O ₃ PbSn	PbO : SnO ₂ -PbZrO ₃	1C-f3	87
O ₃ PbSn	PbO : SnO ₂ -PbHfO ₃ -PbTiO ₃	1C-f18	88
O ₃ PbSn	PbO : SnO ₂ -PbTiO ₃ -PbZrO ₃	5B-6	101
O ₃ PbSn	(Pb-Ba)(Sn-Ti)O ₃	1C-e13	87
O ₆ PbTa ₂	PbTa ₂ O ₆ -PbNb ₂ O ₆	5B-16	102
O ₆ PbTa ₂	PbTa ₂ O ₆ -PbZrO ₃	5B-15	102
O ₆ PbTa ₂	PbTa ₂ O ₆ -SrTa ₂ O ₆	5B-15	102
O ₆ PbTa ₂	(Pb-Ba-Ca)(Ta-Nb) ₂ O ₆	5B-15	102
O ₆ PbTa ₂	(Pb-Ba-Sr)(Ta-Nb) ₂ O ₆	1C-b10	83
O ₆ PbTa ₂	PbTiO ₃ -BaSnO ₃	1C-a11	75
O ₃ PbTi	PbTiO ₃ -BaTiO ₃	1C-b9	82
O ₃ PbTi	PbTiO ₃ -BaZrO ₃	1C-c13	84
O ₃ PbTi	PbTiO ₃ -BiFeO ₃	1C-b6	82
O ₃ PbTi	PbTiO ₃ -CaSnO ₃	1C-a8	75
O ₃ PbTi	PbTiO ₃ -CaTiO ₃	1C-b5	82
O ₃ PbTi	PbTiO ₃ -CaZrO ₃	1C-d5	84
O ₃ PbTi	PbTiO ₃ -(K _{1/2} Bi _{1/2})TiO ₃	1C-c6	83
O ₃ PbTi	PbTiO ₃ -KNbO ₃	1C-c10	84
O ₃ PbTi	PbTiO ₃ -LaAlO ₃	1C-c12	84
O ₃ PbTi	PbTiO ₃ -LaFeO ₃	1C-c11	84
O ₃ PbTi	PbTiO ₃ -LaMnO ₃	1C-d8	85
O ₃ PbTi	PbTiO ₃ -(Li _{1/2} Ce _{1/2})TiO ₃	1C-d6	84
O ₃ PbTi	PbTiO ₃ -(Li _{1/2} La _{1/2})TiO ₃	1C-d9	85
O ₃ PbTi	PbTiO ₃ -(Li _{1/2} Nd _{1/2})TiO ₃	1C-d4	84
O ₃ PbTi	PbTiO ₃ -(Na _{1/2} Bi _{1/2})TiO ₃	1C-d7	85
O ₃ PbTi	PbTiO ₃ -(Na _{1/2} La _{1/2})TiO ₃		

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101	O ₃ PbTi	PbTiO ₃ -NaNbO ₃	1C-c3	83
101	O ₃ PbTi	PbTiO ₃ -Pb(Fe _{1/2} Ta _{1/2})O ₃	1C-d11	85
101	O ₃ PbTi	PbTiO ₃ -PbHfO ₃	1C-a29	82
101	O ₃ PbTi	PbTiO ₃ -Pb(Mg _{1/2} W _{1/2})O ₃	1C-d10	85
86	O ₃ PbTi	PbTiO ₃ -Pb(Mn _{1/2} Nb _{1/2})O ₃	1C-d13	85
101	O ₃ PbTi	PbTiO ₃ -PbNb ₂ O ₆	5B-7	101
101	O ₃ PbTi	PbTiO ₃ -PbO:SnO ₂	1C-a30	82
101	O ₃ PbTi	PbTiO ₃ -Pb(Sc _{1/2} Nb _{1/2})O ₃	1C-d12	85
101	O ₃ PbTi	PbTiO ₃ -PbZrO ₃	1C-a27	77
101	O ₃ PbTi	PbTiO ₃ -SrSnO ₃	1C-b8	82
87	O ₃ PbTi	PbTiO ₃ -SrTiO ₃	1C-a10	75
101	O ₃ PbTi	PbTiO ₃ -SrZrO ₃	1C-b7	82
101	O ₃ PbTi	PbTiO ₃ -ABO ₃ -PbZrO ₃	1C-f9	87
100	O ₃ PbTi	PbTiO ₃ -BaTiO ₃ -CaTiO ₃	1C-f2	87
101	O ₃ PbTi	PbTiO ₃ -BiFeO ₃ -PbZrO ₃	1C-f6	87
102	O ₃ PbTi	PbTiO ₃ -LaCoO ₃ -LaMnO ₃	1C-f11	87
88	O ₃ PbTi	PbTiO ₃ -LaCrO ₃ -LaMnO ₃	1C-f11	87
102	O ₃ PbTi	PbTiO ₃ -LaFeO ₃ -LaMnO ₃	1C-f11	87
102	O ₃ PbTi	PbTiO ₃ -LaFeO ₃ -PbZrO ₃	1C-f5	87
106	O ₃ PbTi	PbTiO ₃ -LaMnO ₃ -LaNiO ₃	1C-f11	87
85	O ₃ PbTi	PbTiO ₃ -LaMnO ₃ -SrTiO ₃	1C-f10	87
85	O ₃ PbTi	PbTiO ₃ -Pb(Fe _{1/2} Nb _{1/2})O ₃ -PbZrO ₃	1C-f8	87
85	O ₃ PbTi	PbTiO ₃ -PbHfO ₃ -PbO:SnO ₂	1C-f4	87
101	O ₃ PbTi	PbTiO ₃ -Pb(Mg _{1/3} Nb _{2/3})O ₃ -PbZrO ₃	1C-f7	87
101	O ₃ PbTi	PbTiO ₃ -PbO:SnO ₂ -PbZrO ₃	1C-f3	87
99	O ₃ PbTi	PbTiO ₃ -BaTiO ₃ -BaNb ₂ O ₆ -PbNb ₂ O ₆	1C-f19	88
103	O ₃ PbTi	(Pb-Ba)(Ti-Sn)O ₃	1C-f18	88
86	O ₃ PbTi	(Pb-Ba)(Ti-Zr)O ₃	1C-f17	88
100	O ₃ PbTi	Pb(Ti-Zr)O ₃	1C-a28	78
102	O ₃ PbTi	(Pb-Sr)(Ti-Zr)O ₃	1C-f16	88
106	O ₃ PbZr	PbZrO ₃ -BaTiO ₃	1C-b3	82
87	O ₃ PbZr	PbZrO ₃ -BaZrO ₃	1C-a15	76
101	O ₃ PbZr	PbZrO ₃ -BiFeO ₃	1C-c14	84
76	O ₃ PbZr	PbZrO ₃ -CaZrO ₃	1C-a13	76
82	O ₃ PbZr	PbZrO ₃ -(K _{1/2} Bi _{1/2})ZrO ₃	1C-d17	85
101	O ₃ PbZr	PbZrO ₃ -(Na _{1/2} Bi _{1/2})TiO ₃	1C-d21	85
82	O ₃ PbZr	PbZrO ₃ -(Na _{1/2} Bi _{1/2})ZrO ₃	1C-d16	85
82	O ₃ PbZr	PbZrO ₃ -NaNbO ₃	1C-c4	83
87	O ₃ PbZr	PbZrO ₃ -Pb(Fe _{1/2} Ta _{1/2})O ₃	1C-d15	85
87	O ₃ PbZr	PbZrO ₃ -PbHfO ₃	1C-a31	82
88	O ₃ PbZr	PbZrO ₃ -PbNb ₂ O ₆	5B-8,	101
101	O ₃ PbZr	PbZrO ₃ -PbO:SnO ₂	1C-e12	87
87	O ₃ PbZr	PbZrO ₃ -Pb(Sc _{1/2} Nb _{1/2})O ₃	1C-a32	82
102	O ₃ PbZr	PbZrO ₃ -PbTa ₂ O ₆	1C-d14	85
102	O ₃ PbZr	PbZrO ₃ -PbTiO ₃	1C-e13	87
102	O ₃ PbZr	PbZrO ₃ -SrZrO ₃	1C-a27	77
83	O ₃ PbZr	Pb(Zr-Ti)O ₃ (PZT)	1C-a14	76
75	O ₃ PbZr	PbZrO ₃ -ABO ₃ -PbTiO ₃	1C-a28	78
82	O ₃ PbZr	PbZrO ₃ -BiFeO ₃ -PbTiO ₃	1C-f9	87
84	O ₃ PbZr	PbZrO ₃ -LaFeO ₃ -PbTiO ₃	1C-f6	87
82	O ₃ PbZr	PbZrO ₃ -Pb(Fe _{1/2} Nb _{1/2})O ₃ -PbTiO ₃	1C-f5	87
75	O ₃ PbZr	PbZrO ₃ -Pb(Mg _{1/3} Nb _{2/3})O ₃ -PbTiO ₃	1C-f8	87
82	O ₃ PbZr	PbZrO ₃ -PbO:SnO ₂ -PbTiO ₃	1C-f7	87
84	O ₃ PbZr	(Pb-Ba)(Zr-Ti)O ₃	1C-f3	87
83	O ₃ PbZr	(Pb-Sr)(Zr-Ti)O ₃	1C-f17	88
84	O ₃ SnSr	SrSnO ₃ -BaSnO ₃	1C-f16	88
84	O ₃ SnSr	SrSnO ₃ -BiFeO ₃	1C-a20	76
84	O ₃ SnSr	SrSnO ₃ -CaSnO ₃	1C-c15	84
84	O ₃ SnSr	SrSnO ₃ -PbTiO ₃	1C-a19	76
85	O ₃ SnSr	SrSnO ₃ -BaSnO ₃ -CaSnO ₃	1C-b8	82
84	O ₆ SrTa ₂	SrTa ₂ O ₆ -PbTa ₂ O ₆	1C-f13	88
85	O ₆ SrTa ₂	(Sr-Ba-Pb)(Ta-Nb) ₂ O ₆	5B-16	102
84	O ₆ SrTa ₂	Sr ₂ Ta ₂ O ₇ -Ca ₂ Ta ₂ O ₇	5B-15	102
85	O ₇ Sr ₂ Ta ₂		6B-6	106

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O ₈ SrTi	SrTiO ₃ -BaTiO ₃	1C-a9	75
O ₃ SrTi	SrTiO ₃ -BiFeO ₃	1C-c7	83
O ₃ SrTi	SrTiO ₃ -Bi ₂ O ₃ · 3TiO ₂	1C-e8	86
O ₃ SrTi	SrTiO ₃ -CaTiO ₃	1C-a6	74
O ₃ SrTi	SrTiO ₃ -PbTiO ₃	1C-a10	75
O ₃ SrTi	SrTiO ₃ -Sr(Fe _{1/2} Ta _{1/2})O ₃	1C-d1	84
O ₃ SrTi	SrTiO ₃ -BaTiO ₃ -CaTiO ₃	1C-f1	87
O ₃ SrTi	SrTiO ₃ -LaMnO ₃ -PbTiO ₃	1C-f10	87
O ₃ SrTi	SrTiO ₃ -BaTiO ₃ -LaInO ₃ -LaYO ₃	1C-f12	88
O ₃ SrZr	(Sr-Pb)(Ti-Zr)O ₃	1C-f16	88
O ₃ SrZr	SrZrO ₃ -PbTiO ₃	1C-b7	82
O ₃ SrZr	SrZrO ₃ -PbZrO ₃	1C-a14	76
O ₃ SrZr	(Sr-Pb)(Zr-Ti)O ₃	1C-f16	88
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